



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:38 PM EDT

PDB ID : 5X41 / pdb_00005x41
Title : 3.5A resolution structure of a cobalt energy-coupling factor transporter using LCP method-CbiMQO
Authors : Bao, Z.; Qi, X.; Zhao, W.; Li, D.; Zhang, P.
Deposited on : 2017-02-09
Resolution : 3.47 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

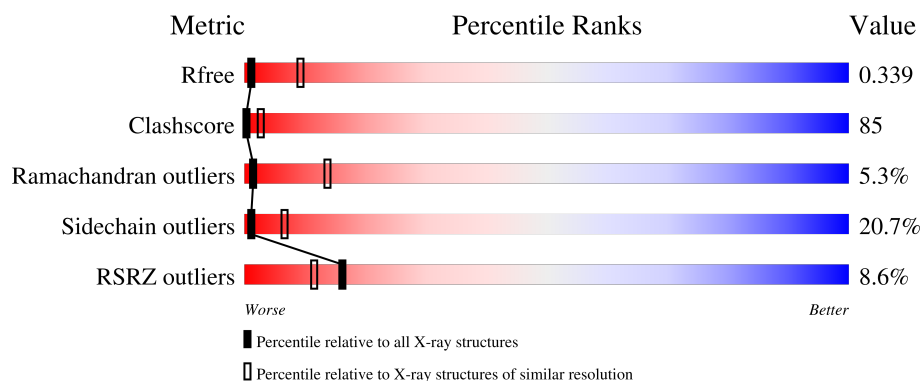
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

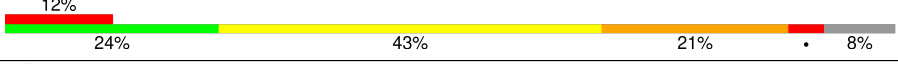
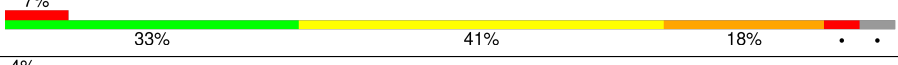
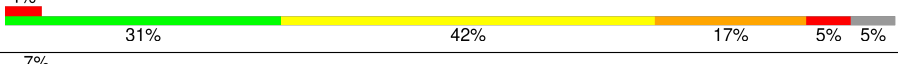
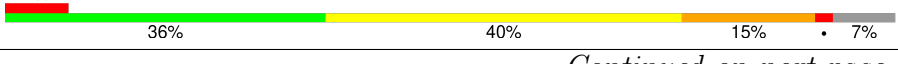
The reported resolution of this entry is 3.47 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	280	
1	B	280	
1	C	280	
1	D	280	
2	E	222	

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Mol	Chain	Length	Quality of chain
2	M	222	5% 41% 41% 9% • 7%
3	F	256	8% 22% 50% 18% 6% 5%
3	Q	256	7% 28% 39% 20% 7% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14359 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cobalt ABC transporter ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			1935	1221	349	362	3			
1	B	258	Total	C	N	O	S	0	0	0
			1899	1197	345	353	4			
1	C	270	Total	C	N	O	S	0	0	0
			1986	1251	362	369	4			
1	D	267	Total	C	N	O	S	0	0	0
			1964	1237	357	366	4			

- Molecule 2 is a protein called Cobalt transport protein CbiM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	207	Total	C	N	O	S	0	0	0
			1470	975	236	252	7			
2	E	207	Total	C	N	O	S	0	0	0
			1470	975	236	252	7			

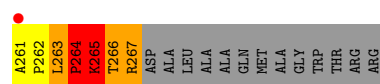
- Molecule 3 is a protein called Uncharacterized protein CbiQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Q	243	Total	C	N	O	S	0	0	0
			1815	1175	333	301	6			
3	F	244	Total	C	N	O	S	0	0	0
			1820	1178	334	302	6			

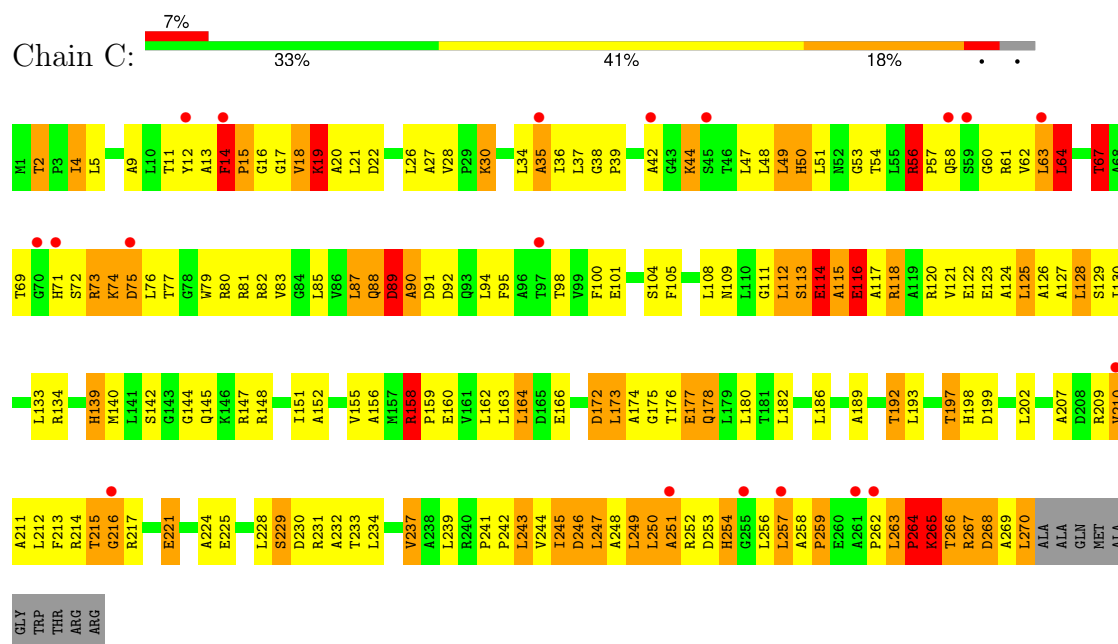
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Chain A:
-
- 14% 20% 41% 27% 6% 6%
- MET THR SER LYS ARG THR HIS GLY P3 I4 L5 E8 A9 T11 Y12 A13 F14 P15 G16 V17 G18 K19 A20 L21 D22 D23 L24 K30 G31 E32 S33 L34 A35 I36 L37 G38 P39 A42 S45 T46 L47 L48 L49 H50 L51 N52 G53 T54 L55 R56 P57 Q58 S59 G60 R61 V62 L63 L64 G65 G66 T67 A68 S129 I130 S131 D132 L133 R134 D135 R136 P137 T138 H139 R140 Y141 L142 S143 G144 R145 K146 R147 R148 A149 V150 A151 A152 G153 A154 V155 A156 M157 R158 P159 E160 V161 L162 L163 L164 D165 E166 P167 T168 A169 D172 L173 A174 G175 T176 E177 Q178 L179 L180 T181 L182 L183 R184 G185 L186 R187 A188 L189 G190 M191 T192 H193 L194 F195 S196 T197 H198 D199 V200 E201 L202 A205 T206 L207 A208 D209 R210 F213 R214 T215 G216 T217 V218 L219 A220 E221 G222 A224 E225 A226 V227 L228 S229 D230 R231 A232 T233 L234 A235 K236 V237 A238 L239 R240 P241 P242 L243 V244 T245 D246 A248 L249 L250 A251

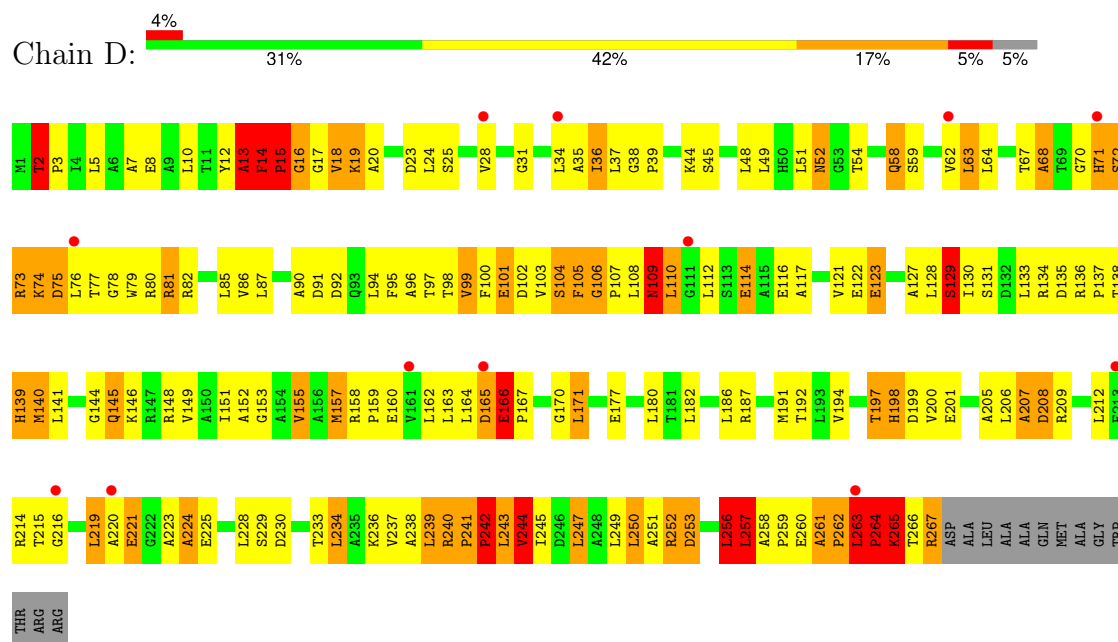
- Chain B:
-
- | Category | Percentage |
|----------|------------|
| H1 | 12% |
| T2 | 24% |
| P3 | 43% |
| I4 | 21% |
| L5 | 8% |
| A6 | 8% |
| A7 | 8% |
| E8 | 8% |
| A9 | 8% |
| L10 | 8% |
| T11 | 8% |
| Y12 | 8% |
| A13 | 8% |
| F14 | 8% |
| P15 | 8% |
| G16 | 8% |
| G17 | 8% |
| V18 | 8% |
| L19 | 8% |
| A20 | 8% |
| L21 | 8% |
| D22 | 8% |
| D23 | 8% |
| L24 | 8% |
| S25 | 8% |
| A27 | 8% |
| V28 | 8% |
| P29 | 8% |
| K30 | 8% |
| E31 | 8% |
| E32 | 8% |
| S33 | 8% |
| L34 | 8% |
| A35 | 8% |
| L36 | 8% |
| L37 | 8% |
| G38 | 8% |
| P39 | 8% |
| N40 | 8% |
| G41 | 8% |
| A42 | 8% |
| G43 | 8% |
| K44 | 8% |
| S45 | 8% |
| L49 | 8% |
| H50 | 8% |
| L51 | 8% |
| N52 | 8% |
| G53 | 8% |
| T54 | 8% |
| L55 | 8% |
| S56 | 8% |
| P57 | 8% |
| Q58 | 8% |
| S59 | 8% |
| G60 | 8% |
| R61 | 8% |
| V62 | 8% |



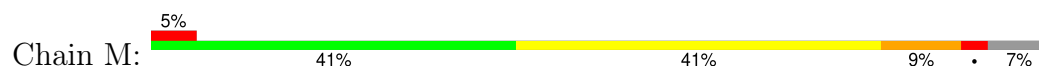
• Molecule 1: Cobalt ABC transporter ATP-binding protein

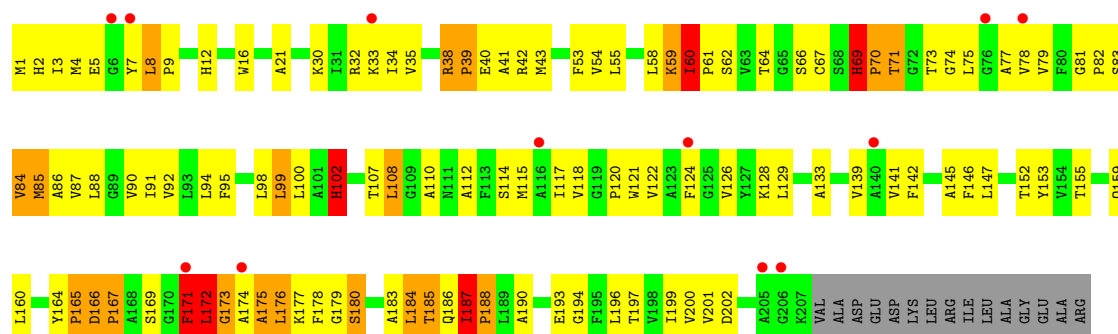


• Molecule 1: Cobalt ABC transporter ATP-binding protein

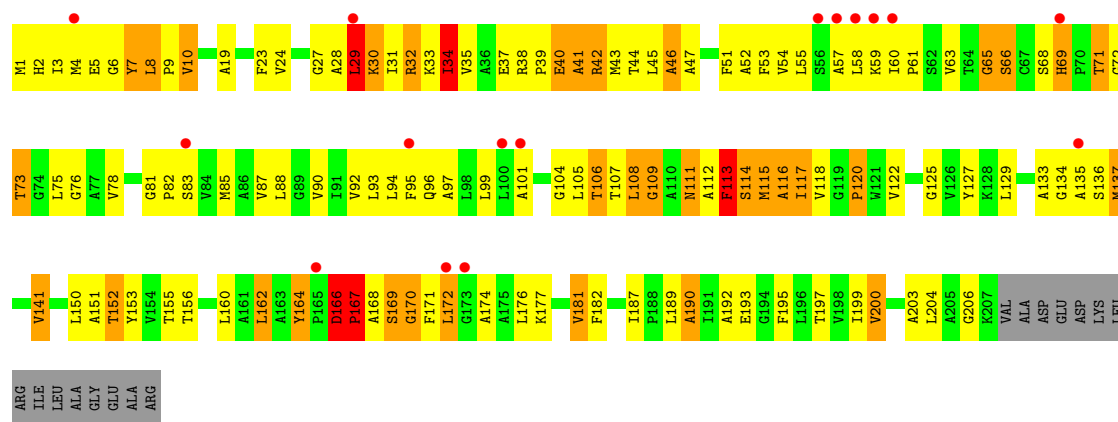


• Molecule 2: Cobalt transport protein CbiM

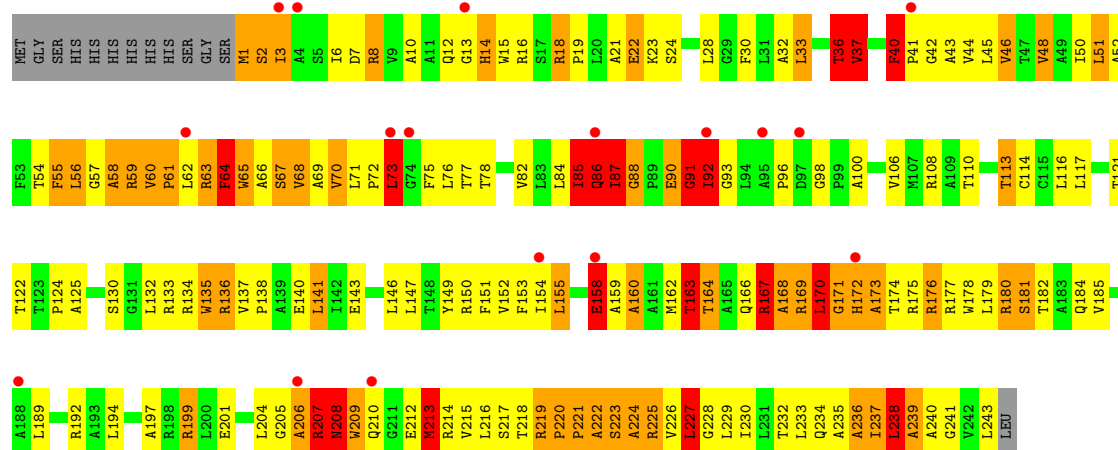




• Molecule 2: Cobalt transport protein CbiM



• Molecule 3: Uncharacterized protein CbiQ



• Molecule 3: Uncharacterized protein CbiQ



I186	A187	A188	L189	P191	R192	A193	L194	T195	R196	A197	R198	R199	L200	E201	T202	G203	L204	G205	A206	R207	N208	W209	Q210	G211	E212	M213	R214	V215	L216	S217	T218	R219	P220	P221	A222	S223	A224	R225	V226	L227	G228	L229	T232	L233	Q234	A235	A236	T237	L238	A239	A240	G241	V242	L243	L244				
T123	P124	A125	A126	D127	L128	L129	S130	G131	L132	R133	R134	V137	P138	A139	E140	L141	T142	E143	I144	A145	L146	L147	T148	Y149	R150	F151	V152	F153	I154	L155	E158	A159	M162	T163	T164	A165	Q166	R167	A168	R169	L170	G171	H172	A173	T174	R175	R176	R177	W178	L179	R180	S181	T182	A183	Q184	V185			
F55	L56	G57	A58	R59	V60		F64	W65	A66	S67	V68	A69	V70	L71	P72	L73	G74	F75	L76	T77	T78	G79	A80	A81	W82	L83	R84	I85	Q86	T87	G88	P89	E90	G91	I92	G93	L94	A95	P96	D97	G98	P99	A100		L105	V106	M107	R108	A109	T110	A111		C114	C115	L116	L117	F118		T122
MET	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	GLY	SER	M1	S2	I3	A4	S5	I6	D7	R8		A11		H14	W15	R16	S17	R18		E22	K23	S24		L28	G29	F30	L31	A32	L33	A34	V35	T36	V37	P38	P39	F40	P41	G42	A43	V44	L45	V46	T47	V48	A49	I50	L51	A52	F53	T54

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.16Å 135.04Å 204.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.96 – 3.47 47.96 – 3.47	Depositor EDS
% Data completeness (in resolution range)	97.5 (47.96-3.47) 97.4 (47.96-3.47)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.299 , 0.335 0.308 , 0.339	Depositor DCC
R_{free} test set	1733 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	99.3	Xtriage
Anisotropy	0.800	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	14359	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.95	5/1960 (0.3%)	1.52	56/2665 (2.1%)
1	B	0.83	2/1923 (0.1%)	1.53	42/2611 (1.6%)
1	C	0.99	8/2013 (0.4%)	1.61	61/2736 (2.2%)
1	D	0.98	6/1990 (0.3%)	1.61	55/2704 (2.0%)
2	E	0.95	1/1504 (0.1%)	1.52	31/2055 (1.5%)
2	M	0.87	4/1504 (0.3%)	1.42	24/2055 (1.2%)
3	F	1.00	4/1855 (0.2%)	1.72	58/2532 (2.3%)
3	Q	1.04	11/1850 (0.6%)	1.66	52/2525 (2.1%)
All	All	0.96	41/14599 (0.3%)	1.58	379/19883 (1.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	6
1	D	0	1
2	E	0	4
2	M	0	1
3	F	0	8
3	Q	0	13
All	All	0	39

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	242	PRO	N-CD	13.64	1.66	1.47
1	C	14	PHE	C-N	8.80	1.40	1.33
3	Q	170	LEU	CA-C	-8.09	1.43	1.53
1	A	106	GLY	C-N	6.80	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	14	PHE	C-N	6.68	1.40	1.34
1	D	240	ARG	C-N	6.56	1.41	1.33
1	C	56	ARG	C-N	6.52	1.41	1.33
3	F	219	ARG	C-N	6.42	1.41	1.33
3	Q	219	ARG	C-N	6.35	1.40	1.33
2	M	69	HIS	CG-ND1	-6.27	1.31	1.38
1	A	263	LEU	C-N	6.21	1.41	1.33
3	F	89	PRO	N-CD	5.77	1.55	1.47
3	Q	37	VAL	C-N	5.70	1.40	1.33
3	Q	41	PRO	N-CD	5.68	1.55	1.47
1	C	38	GLY	C-N	5.67	1.40	1.33
3	Q	209	TRP	CA-C	-5.64	1.45	1.52
1	B	241	PRO	C-N	5.63	1.40	1.33
3	Q	137	VAL	C-N	5.60	1.40	1.33
1	C	57	PRO	N-CD	5.41	1.55	1.47
1	A	107	PRO	N-CD	5.41	1.55	1.47
1	B	241	PRO	N-CD	5.33	1.55	1.47
1	C	39	PRO	N-CD	5.33	1.55	1.47
3	Q	206	ALA	C-N	5.33	1.40	1.33
2	M	167	PRO	N-CD	5.32	1.55	1.47
2	M	166	ASP	C-N	5.31	1.40	1.33
1	C	159	PRO	N-CD	5.31	1.55	1.47
3	Q	60	VAL	CA-C	-5.18	1.49	1.52
2	M	188	PRO	N-CD	5.18	1.54	1.47
1	D	259	PRO	N-CD	5.15	1.54	1.47
1	C	115	ALA	N-CA	-5.15	1.40	1.47
2	E	106	THR	C-O	5.13	1.30	1.24
1	D	264	PRO	N-CD	5.10	1.54	1.47
3	Q	61	PRO	N-CD	5.08	1.54	1.47
1	A	137	PRO	N-CD	5.07	1.54	1.47
3	F	41	PRO	N-CD	5.05	1.54	1.47
1	D	15	PRO	N-CD	5.05	1.54	1.47
3	Q	220	PRO	N-CD	5.03	1.54	1.47
1	C	15	PRO	N-CD	5.03	1.54	1.47
3	F	220	PRO	N-CD	5.03	1.54	1.47
1	A	259	PRO	N-CD	5.02	1.54	1.47
3	Q	138	PRO	N-CD	5.01	1.54	1.47

All (379) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	139	ALA	N-CA-C	19.86	135.63	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	79	VAL	N-CA-C	19.19	128.20	110.74
2	E	10	VAL	N-CA-C	18.29	128.04	110.30
3	Q	173	ALA	N-CA-C	17.05	129.55	110.97
3	Q	207	ARG	N-CA-C	-16.24	89.58	110.53
2	E	166	ASP	CA-C-N	15.79	139.58	119.84
2	E	166	ASP	C-N-CA	15.79	139.58	119.84
3	Q	92	ILE	CB-CA-C	15.50	133.34	111.80
3	F	2	SER	N-CA-CB	-15.43	87.39	109.91
3	Q	207	ARG	N-CA-CB	-14.75	89.35	110.44
1	A	9	ALA	N-CA-C	-14.56	88.46	110.30
1	B	221	GLU	N-CA-C	14.35	132.10	111.87
2	M	79	VAL	CB-CA-C	-13.04	94.72	111.94
1	D	205	ALA	CB-CA-C	12.93	131.33	110.90
1	C	64	LEU	CB-CA-C	-12.72	89.59	110.19
3	F	71	LEU	CA-C-N	-12.65	106.78	119.56
3	F	71	LEU	C-N-CA	-12.65	106.78	119.56
1	C	64	LEU	N-CA-C	12.33	128.83	108.73
3	F	82	VAL	CB-CA-C	-12.17	99.19	110.63
3	F	139	ALA	CB-CA-C	-12.02	90.61	110.79
3	Q	92	ILE	N-CA-C	-11.67	91.77	107.88
1	C	20	ALA	N-CA-C	11.63	127.65	113.12
1	D	130	ILE	N-CA-C	-11.55	99.76	111.77
3	Q	92	ILE	CA-C-N	11.52	144.00	121.41
3	Q	92	ILE	C-N-CA	11.52	144.00	121.41
3	F	58	ALA	CB-CA-C	11.51	130.23	109.29
1	D	14	PHE	N-CA-C	11.32	134.84	109.81
3	Q	207	ARG	CB-CA-C	11.05	133.28	110.40
3	Q	173	ALA	N-CA-CB	-10.90	93.99	109.91
1	D	258	ALA	N-CA-C	10.90	120.89	108.25
1	D	224	ALA	N-CA-C	10.88	122.83	110.97
3	Q	172	HIS	N-CA-C	10.84	127.83	113.30
1	B	95	PHE	N-CA-C	10.73	125.08	111.24
1	D	221	GLU	N-CA-C	10.73	127.05	110.42
3	F	172	HIS	N-CA-C	-10.73	90.92	108.41
1	B	14	PHE	CB-CA-C	10.64	124.18	108.86
1	C	264	PRO	N-CA-C	-10.64	90.56	112.47
1	D	221	GLU	N-CA-CB	-10.58	94.05	110.56
1	B	60	GLY	N-CA-C	-10.50	91.47	111.01
1	B	109	ASN	N-CA-C	-10.47	100.79	112.72
1	C	19	LYS	CB-CA-C	-10.36	97.84	111.42
1	D	165	ASP	N-CA-C	-10.25	97.47	110.19
2	M	185	THR	N-CA-CB	-10.05	94.62	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	ALA	CB-CA-C	-10.03	94.80	111.24
1	C	49	LEU	CA-C-N	10.01	134.99	120.38
1	C	49	LEU	C-N-CA	10.01	134.99	120.38
1	D	205	ALA	N-CA-C	-9.74	100.62	111.14
1	D	206	LEU	N-CA-CB	-9.73	94.95	110.14
3	Q	13	GLY	N-CA-C	-9.66	97.18	111.19
3	F	68	VAL	CB-CA-C	-9.56	99.42	112.24
1	B	66	GLY	N-CA-C	9.35	135.33	113.18
1	D	241	PRO	N-CA-C	-9.34	99.31	110.70
3	F	140	GLU	N-CA-CB	-9.31	95.43	110.14
3	Q	14	HIS	N-CA-C	9.30	123.89	112.54
3	Q	73	LEU	CB-CA-C	-9.08	92.36	110.42
1	C	19	LYS	N-CA-C	9.01	122.28	107.23
3	F	111	ALA	N-CA-C	9.01	120.79	110.97
3	Q	137	VAL	CA-C-N	-8.98	111.59	120.21
3	Q	137	VAL	C-N-CA	-8.98	111.59	120.21
3	F	59	ARG	N-CA-CB	8.86	125.94	112.47
1	A	93	GLN	N-CA-CB	-8.83	98.39	110.67
1	D	242	PRO	CA-N-CD	-8.81	99.66	112.00
3	F	40	PHE	C-N-CD	8.81	139.99	120.60
1	D	106	GLY	O-C-N	8.80	124.24	121.07
3	F	88	GLY	N-CA-C	8.76	130.21	112.34
1	D	256	LEU	N-CA-C	8.75	120.82	111.28
2	E	10	VAL	CB-CA-C	-8.75	100.87	111.81
1	B	94	LEU	CB-CA-C	-8.63	97.18	111.51
1	D	157	MET	N-CA-C	-8.63	97.74	110.52
2	E	113	PHE	N-CA-C	8.61	120.67	111.28
1	D	109	ASN	N-CA-C	-8.58	103.32	112.93
3	F	38	PRO	CB-CA-C	-8.56	100.47	110.92
1	C	30	LYS	N-CA-C	8.55	123.27	113.01
3	F	209	TRP	CB-CA-C	-8.53	95.67	109.75
1	A	106	GLY	CA-C-N	-8.39	109.74	119.05
1	A	106	GLY	C-N-CA	-8.39	109.74	119.05
1	B	215	THR	N-CA-C	-8.33	93.06	110.80
1	B	228	LEU	CB-CA-C	8.27	126.88	110.42
1	A	109	ASN	N-CA-C	-8.19	102.35	111.28
2	M	117	ILE	N-CA-C	8.13	118.80	111.81
3	Q	64	PHE	N-CA-C	8.12	124.18	113.30
1	D	198	HIS	N-CA-C	-8.06	102.50	113.30
1	C	210	VAL	CB-CA-C	-8.06	99.16	110.12
1	B	206	LEU	N-CA-CB	-8.02	100.33	111.00
1	B	157	MET	N-CA-C	-8.02	99.94	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	165	ASP	CB-CA-C	8.01	129.16	111.30
1	A	58	GLN	N-CA-C	-7.89	101.98	111.69
3	F	88	GLY	C-N-CD	7.89	137.97	120.60
1	C	60	GLY	N-CA-C	-7.86	103.49	112.29
1	D	171	LEU	N-CA-C	7.85	121.31	110.24
1	C	94	LEU	N-CA-C	7.83	121.84	107.99
1	D	207	ALA	CB-CA-C	-7.79	97.76	110.77
1	B	82	ARG	N-CA-C	7.76	119.82	111.36
2	M	184	LEU	CB-CA-C	7.74	126.49	110.31
1	C	94	LEU	CB-CA-C	-7.70	98.23	110.79
1	A	76	LEU	CB-CA-C	-7.67	97.46	109.80
2	E	170	GLY	N-CA-C	-7.64	100.77	112.84
1	C	9	ALA	N-CA-CB	7.64	123.39	110.49
1	B	241	PRO	CA-C-N	-7.59	112.92	120.21
1	B	241	PRO	C-N-CA	-7.59	112.92	120.21
1	A	4	ILE	CB-CA-C	7.55	121.46	111.94
3	Q	37	VAL	CA-C-N	-7.53	112.62	120.38
3	Q	37	VAL	C-N-CA	-7.53	112.62	120.38
1	B	67	THR	N-CA-CB	7.46	124.04	110.76
2	E	7	TYR	N-CA-C	-7.44	101.43	113.19
1	A	108	LEU	CA-C-N	7.44	130.24	120.28
1	A	108	LEU	C-N-CA	7.44	130.24	120.28
1	D	207	ALA	N-CA-C	7.42	120.17	108.67
3	F	70	VAL	N-CA-C	7.31	117.29	110.42
1	B	94	LEU	N-CA-C	7.28	123.21	107.49
2	E	8	LEU	CA-C-N	7.26	128.91	119.84
2	E	8	LEU	C-N-CA	7.26	128.91	119.84
1	C	210	VAL	N-CA-C	7.23	118.55	107.78
1	A	224	ALA	N-CA-C	-7.20	103.36	111.07
1	D	240	ARG	CA-C-N	-7.19	112.97	120.38
1	D	240	ARG	C-N-CA	-7.19	112.97	120.38
3	F	49	ALA	N-CA-C	-7.16	103.40	111.07
1	D	14	PHE	CA-C-N	-7.14	112.83	120.47
1	D	14	PHE	C-N-CA	-7.14	112.83	120.47
2	E	106	THR	CA-C-O	7.11	128.02	120.70
2	M	99	LEU	N-CA-C	7.10	122.26	112.04
1	C	67	THR	N-CA-C	-7.05	97.46	109.24
1	B	140	MET	N-CA-C	-7.03	101.24	111.30
2	E	29	LEU	CA-C-N	-7.03	110.95	122.54
2	E	29	LEU	C-N-CA	-7.03	110.95	122.54
1	D	129	SER	CB-CA-C	-7.01	99.94	111.36
2	M	59	LYS	CA-CB-CG	-7.00	100.09	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	71	THR	N-CA-C	-6.98	97.87	109.46
1	D	171	LEU	CB-CA-C	-6.97	98.48	109.70
1	C	87	LEU	N-CA-C	6.96	120.69	110.17
1	D	206	LEU	CB-CA-C	6.93	124.00	111.03
3	F	124	PRO	CA-C-O	6.92	129.23	121.34
2	M	38	ARG	CA-C-N	6.91	128.47	119.84
2	M	38	ARG	C-N-CA	6.91	128.47	119.84
3	F	18	ARG	CA-C-N	6.88	128.44	119.84
3	F	18	ARG	C-N-CA	6.88	128.44	119.84
3	Q	206	ALA	N-CA-C	-6.87	102.64	111.02
1	B	238	ALA	CB-CA-C	-6.86	100.24	110.67
3	Q	219	ARG	CA-C-N	-6.85	113.33	120.38
3	Q	219	ARG	C-N-CA	-6.85	113.33	120.38
3	F	219	ARG	CA-C-N	-6.85	113.33	120.38
3	F	219	ARG	C-N-CA	-6.85	113.33	120.38
1	A	107	PRO	CA-N-CD	-6.84	102.42	112.00
1	B	139	HIS	CB-CA-C	-6.83	97.39	110.57
3	F	140	GLU	N-CA-C	6.81	120.47	111.75
1	D	36	ILE	CB-CA-C	-6.81	105.59	113.22
1	C	265	LYS	N-CA-C	-6.80	100.96	110.35
3	F	111	ALA	CB-CA-C	-6.80	100.48	110.96
1	C	22	ASP	N-CA-C	6.79	121.86	107.67
1	C	38	GLY	CA-C-N	-6.78	113.81	120.52
1	C	38	GLY	C-N-CA	-6.78	113.81	120.52
1	D	14	PHE	N-CA-CB	-6.76	98.34	110.37
1	D	239	LEU	CB-CA-C	-6.75	98.34	110.36
1	A	221	GLU	N-CA-C	6.73	118.42	108.60
2	M	187	ILE	CA-C-N	-6.67	111.50	119.84
2	M	187	ILE	C-N-CA	-6.67	111.50	119.84
1	A	130	ILE	N-CA-C	-6.66	102.68	110.21
1	A	215	THR	N-CA-C	-6.63	96.68	110.80
1	B	184	ARG	N-CA-C	-6.62	104.14	111.36
3	F	46	VAL	CB-CA-C	-6.62	103.21	112.14
1	A	263	LEU	CA-C-N	-6.61	112.69	119.83
1	A	263	LEU	C-N-CA	-6.61	112.69	119.83
1	B	41	GLY	N-CA-C	-6.61	105.95	115.27
3	F	173	ALA	N-CA-C	-6.60	96.74	110.80
2	M	38	ARG	N-CA-CB	-6.58	101.92	111.20
1	A	222	GLY	N-CA-C	6.54	124.34	115.32
3	Q	98	GLY	CA-C-N	6.53	128.00	119.84
3	Q	98	GLY	C-N-CA	6.53	128.00	119.84
3	Q	36	THR	N-CA-C	6.50	118.16	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	81	GLY	CA-C-N	-6.50	112.21	118.97
2	M	81	GLY	C-N-CA	-6.50	112.21	118.97
1	C	35	ALA	CA-C-N	-6.48	115.08	122.93
1	C	35	ALA	C-N-CA	-6.48	115.08	122.93
2	E	82	PRO	N-CA-CB	-6.47	96.46	103.25
1	B	5	LEU	N-CA-CB	-6.44	100.85	110.90
1	C	174	ALA	N-CA-C	-6.44	104.18	111.14
1	A	100	PHE	CA-C-N	-6.44	112.07	120.44
1	A	100	PHE	C-N-CA	-6.44	112.07	120.44
3	Q	85	ILE	N-CA-C	6.42	122.70	109.34
3	Q	18	ARG	CA-C-N	6.42	127.86	119.84
3	Q	18	ARG	C-N-CA	6.42	127.86	119.84
1	A	229	SER	CB-CA-C	-6.40	98.63	109.38
1	C	95	PHE	N-CA-CB	-6.39	101.35	110.81
1	D	224	ALA	CB-CA-C	-6.39	101.12	110.96
1	B	91	ASP	N-CA-C	-6.38	105.36	113.02
1	C	14	PHE	CA-C-N	-6.38	113.32	121.04
1	C	14	PHE	C-N-CA	-6.38	113.32	121.04
1	B	205	ALA	CB-CA-C	6.38	119.73	109.02
1	B	108	LEU	N-CA-C	6.35	119.50	111.69
1	A	94	LEU	CB-CA-C	-6.34	101.03	111.68
3	Q	213	MET	N-CA-CB	6.33	121.19	110.49
1	C	211	ALA	N-CA-CB	-6.33	100.25	110.69
1	C	90	ALA	N-CA-C	-6.30	106.23	114.04
1	D	244	VAL	CB-CA-C	-6.29	103.54	112.22
1	C	264	PRO	CB-CA-C	6.28	121.92	111.56
1	A	108	LEU	N-CA-C	6.27	119.09	111.82
1	C	56	ARG	CA-C-N	-6.25	113.06	120.13
1	C	56	ARG	C-N-CA	-6.25	113.06	120.13
3	F	68	VAL	N-CA-C	6.25	117.81	111.00
1	A	58	GLN	CB-CA-C	6.24	122.11	110.70
3	F	133	ARG	N-CA-C	6.22	118.86	111.71
1	A	33	SER	N-CA-CB	-6.22	100.65	110.79
1	A	187	ARG	N-CA-C	-6.21	104.51	111.28
1	A	10	LEU	CB-CA-C	-6.18	98.18	109.54
3	F	178	TRP	N-CA-C	-6.18	104.45	112.23
2	M	7	TYR	N-CA-C	-6.17	105.33	112.92
3	F	56	LEU	N-CA-C	-6.16	104.49	111.14
1	D	241	PRO	CB-CA-C	6.14	118.41	110.92
1	D	16	GLY	N-CA-C	6.13	120.08	112.73
1	C	57	PRO	CB-CA-C	-6.12	103.94	111.11
3	F	168	ALA	N-CA-C	-6.11	101.43	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	49	LEU	N-CA-C	6.11	118.74	111.71
1	C	262	PRO	CA-N-CD	-6.11	103.45	112.00
1	C	30	LYS	CB-CA-C	-6.10	97.73	110.17
3	F	58	ALA	N-CA-CB	-6.09	101.57	110.53
1	C	268	ASP	N-CA-C	6.08	118.42	109.24
1	A	94	LEU	N-CA-C	6.08	119.40	107.98
2	E	109	GLY	N-CA-C	-6.02	105.50	112.73
1	A	167	PRO	N-CA-C	-6.02	106.82	114.35
3	F	41	PRO	CA-N-CD	-6.02	103.07	111.50
2	M	98	LEU	CB-CA-C	6.01	120.40	110.90
1	C	49	LEU	CB-CA-C	-6.01	99.51	110.63
3	F	225	ARG	N-CA-CB	-6.00	101.32	110.26
1	C	114	GLU	N-CA-C	5.98	120.65	112.04
1	C	139	HIS	N-CA-C	-5.96	104.39	112.26
3	Q	58	ALA	CA-C-N	-5.96	112.53	121.05
3	Q	58	ALA	C-N-CA	-5.96	112.53	121.05
1	D	106	GLY	CA-C-N	5.95	127.28	119.84
1	D	106	GLY	C-N-CA	5.95	127.28	119.84
3	F	97	ASP	N-CA-CB	-5.94	98.73	110.48
1	A	95	PHE	N-CA-C	5.92	123.42	110.80
3	Q	73	LEU	N-CA-C	5.92	123.42	110.80
3	F	176	ARG	N-CA-CB	-5.92	101.61	110.60
3	F	209	TRP	N-CA-CB	5.90	120.05	110.43
1	D	110	LEU	N-CA-C	-5.90	105.91	112.57
3	F	3	ILE	N-CA-C	5.89	116.54	110.82
1	C	259	PRO	CA-N-CD	-5.89	103.75	112.00
3	F	57	GLY	N-CA-C	-5.86	99.29	113.18
1	D	105	PHE	N-CA-C	5.86	117.66	111.28
1	A	175	GLY	N-CA-C	-5.83	105.73	112.73
1	A	100	PHE	N-CA-C	-5.83	104.93	111.28
1	C	211	ALA	N-CA-C	5.83	119.40	107.69
3	F	224	ALA	CB-CA-C	5.83	122.01	110.42
1	B	195	PHE	N-CA-C	5.81	117.95	108.55
1	C	144	GLY	N-CA-C	-5.80	107.47	114.66
1	A	259	PRO	CA-N-CD	-5.80	103.88	112.00
1	C	22	ASP	N-CA-CB	-5.79	100.25	110.90
1	A	147	ARG	N-CA-C	-5.78	104.98	111.28
3	Q	213	MET	N-CA-C	5.77	123.10	110.80
1	A	15	PRO	CA-N-CD	-5.77	103.92	112.00
1	B	233	THR	N-CA-C	-5.76	105.00	111.28
1	A	97	THR	N-CA-C	5.75	117.35	111.14
2	E	190	ALA	N-CA-C	-5.75	105.02	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	LEU	N-CA-CB	-5.73	102.13	110.84
1	A	13	ALA	N-CA-C	-5.73	100.36	109.07
1	A	201	GLU	N-CA-C	-5.72	104.24	111.11
2	E	71	THR	CB-CA-C	5.72	119.17	109.80
3	Q	65	TRP	N-CA-C	-5.70	105.07	111.28
1	A	104	SER	N-CA-C	-5.69	105.08	111.28
2	E	187	ILE	CA-C-N	-5.68	113.82	119.56
2	E	187	ILE	C-N-CA	-5.68	113.82	119.56
2	E	29	LEU	CA-CB-CG	5.68	136.17	116.30
3	Q	45	LEU	N-CA-C	-5.68	106.40	113.38
1	D	166	GLU	N-CA-C	-5.66	102.61	109.57
3	Q	155	LEU	N-CA-C	-5.66	107.62	114.75
2	M	166	ASP	CA-C-N	-5.64	113.08	119.28
2	M	166	ASP	C-N-CA	-5.64	113.08	119.28
3	Q	163	THR	N-CA-C	-5.63	105.14	111.28
1	B	108	LEU	CB-CA-C	-5.63	100.40	110.70
3	F	208	ASN	N-CA-CB	-5.63	100.98	110.49
1	D	219	LEU	N-CA-C	5.61	117.26	111.03
1	C	172	ASP	CB-CA-C	-5.61	97.97	110.19
1	B	266	THR	N-CA-C	-5.58	104.69	112.45
3	F	169	ARG	CB-CA-C	-5.58	110.13	116.54
1	D	2	THR	CA-C-N	5.55	125.46	119.85
1	D	2	THR	C-N-CA	5.55	125.46	119.85
1	C	89	ASP	N-CA-C	-5.53	99.02	110.80
3	F	70	VAL	CB-CA-C	-5.52	104.75	111.87
1	A	174	ALA	N-CA-C	-5.52	104.90	111.69
1	D	68	ALA	N-CA-C	5.50	118.45	109.59
1	B	264	PRO	CA-N-CD	-5.50	104.30	112.00
3	Q	86	GLN	N-CA-CB	5.49	118.39	110.37
2	E	122	VAL	N-CA-C	-5.48	105.27	110.42
1	C	114	GLU	CA-C-N	5.48	131.04	123.04
1	C	114	GLU	C-N-CA	5.48	131.04	123.04
1	B	263	LEU	CA-C-N	-5.47	113.01	119.84
1	B	263	LEU	C-N-CA	-5.47	113.01	119.84
1	A	251	ALA	N-CA-C	-5.46	105.33	111.28
1	D	263	LEU	CA-C-N	-5.46	113.02	119.84
1	D	263	LEU	C-N-CA	-5.46	113.02	119.84
3	Q	167	ARG	N-CA-C	-5.45	105.23	111.07
3	F	75	PHE	N-CA-C	-5.45	106.76	113.41
3	F	52	ALA	N-CA-C	-5.45	105.34	111.28
3	F	237	ILE	N-CA-C	-5.44	98.03	109.34
1	D	109	ASN	N-CA-CB	5.42	118.03	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	13	ALA	N-CA-C	-5.41	100.22	108.76
1	C	118	ARG	N-CA-C	-5.40	105.39	111.28
1	B	90	ALA	CB-CA-C	-5.40	98.39	110.21
2	M	60	ILE	N-CA-C	-5.40	104.76	109.19
1	A	154	ALA	CA-C-N	5.39	129.48	120.64
1	A	154	ALA	C-N-CA	5.39	129.48	120.64
1	B	96	ALA	N-CA-C	5.37	119.24	111.56
1	A	52	ASN	N-CA-C	5.37	118.94	112.93
2	E	73	THR	N-CA-CB	-5.37	103.76	110.90
1	A	4	ILE	N-CA-C	-5.37	105.89	111.58
3	Q	220	PRO	CA-C-N	-5.37	113.13	119.84
3	Q	220	PRO	C-N-CA	-5.37	113.13	119.84
1	B	2	THR	CA-C-N	5.36	125.30	119.78
1	B	2	THR	C-N-CA	5.36	125.30	119.78
1	B	77	THR	N-CA-C	-5.36	105.44	111.28
1	D	81	ARG	CA-C-N	5.35	129.78	120.68
1	D	81	ARG	C-N-CA	5.35	129.78	120.68
3	F	174	THR	CB-CA-C	-5.35	99.78	110.42
3	Q	64	PHE	O-C-N	5.35	128.71	122.24
2	E	167	PRO	CA-N-CD	-5.33	104.53	112.00
3	Q	40	PHE	O-C-N	5.33	125.22	120.48
3	F	227	LEU	N-CA-C	-5.32	107.34	113.88
1	B	14	PHE	N-CA-C	-5.30	102.97	110.29
1	C	164	LEU	CA-C-N	-5.30	115.72	122.77
1	C	164	LEU	C-N-CA	-5.30	115.72	122.77
3	Q	40	PHE	CA-C-N	-5.30	113.17	119.05
3	Q	40	PHE	C-N-CA	-5.30	113.17	119.05
3	Q	67	SER	N-CA-C	-5.29	105.51	111.28
1	B	65	GLY	CA-C-N	5.28	131.76	121.41
1	B	65	GLY	C-N-CA	5.28	131.76	121.41
1	A	14	PHE	CA-C-N	-5.27	113.26	119.84
1	A	14	PHE	C-N-CA	-5.27	113.26	119.84
1	C	88	GLN	N-CA-C	-5.26	100.59	108.96
2	E	81	GLY	CA-C-N	5.26	126.42	119.84
2	E	81	GLY	C-N-CA	5.26	126.42	119.84
2	E	41	ALA	N-CA-C	-5.26	105.55	111.28
3	F	16	ARG	N-CA-C	-5.26	105.63	111.36
3	Q	160	ALA	N-CA-C	-5.25	105.56	111.28
1	C	20	ALA	N-CA-CB	-5.22	102.43	110.42
1	C	166	GLU	CA-C-N	-5.22	113.25	119.05
1	C	166	GLU	C-N-CA	-5.22	113.25	119.05
3	F	124	PRO	N-CA-C	5.22	119.28	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	ARG	CA-C-N	-5.22	113.32	119.84
1	C	158	ARG	C-N-CA	-5.22	113.32	119.84
2	M	21	ALA	CA-C-N	-5.21	114.30	119.56
2	M	21	ALA	C-N-CA	-5.21	114.30	119.56
1	A	38	GLY	CA-C-N	5.20	125.18	120.03
1	A	38	GLY	C-N-CA	5.20	125.18	120.03
3	Q	60	VAL	CA-C-N	-5.20	113.28	119.05
3	Q	60	VAL	C-N-CA	-5.20	113.28	119.05
3	F	206	ALA	CB-CA-C	5.19	120.74	110.42
1	D	58	GLN	N-CA-C	-5.18	106.95	113.28
1	A	263	LEU	N-CA-C	-5.18	102.74	110.20
1	A	136	ARG	CA-C-N	-5.17	113.37	119.84
1	A	136	ARG	C-N-CA	-5.17	113.37	119.84
1	C	4	ILE	N-CA-C	-5.17	108.25	113.47
2	M	59	LYS	N-CA-C	5.17	118.16	110.14
3	Q	100	ALA	N-CA-C	-5.17	105.81	112.68
1	C	123	GLU	CB-CA-C	5.16	120.90	110.38
1	C	116	GLU	N-CA-C	-5.16	105.66	111.28
1	D	108	LEU	CA-C-N	-5.15	114.10	122.65
1	D	108	LEU	C-N-CA	-5.15	114.10	122.65
3	F	40	PHE	CA-C-N	-5.15	114.64	127.00
3	F	40	PHE	C-N-CA	-5.15	114.64	127.00
1	A	120	ARG	N-CA-C	-5.12	108.05	114.56
1	B	17	GLY	N-CA-C	5.12	120.61	110.83
3	Q	146	LEU	N-CA-C	-5.11	106.56	112.89
1	A	9	ALA	CB-CA-C	5.10	117.15	110.06
3	Q	208	ASN	N-CA-C	-5.09	106.28	113.20
1	A	149	VAL	CB-CA-C	-5.09	105.27	112.14
2	M	180	SER	N-CA-CB	-5.09	103.82	110.59
2	E	46	ALA	N-CA-C	-5.07	105.75	111.28
1	D	145	GLN	N-CA-C	5.07	117.54	111.71
3	F	90	GLU	N-CA-C	-5.06	105.77	111.28
3	F	34	ALA	N-CA-C	-5.05	105.77	111.28
2	M	102	HIS	N-CA-CB	-5.04	103.11	110.47
1	D	257	LEU	N-CA-C	5.04	116.80	108.49
1	C	75	ASP	N-CA-C	-5.03	107.09	114.39
3	F	2	SER	N-CA-C	5.03	116.45	110.97
1	B	247	LEU	N-CA-C	5.03	117.26	108.76
2	E	164	TYR	CA-C-N	-5.03	113.56	119.84
2	E	164	TYR	C-N-CA	-5.03	113.56	119.84
3	Q	158	GLU	N-CA-C	-5.01	105.90	111.36
2	E	166	ASP	C-N-CD	-5.00	104.49	125.00

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	ASP	Peptide
1	A	216	GLY	Peptide
1	B	223	ALA	Peptide
1	B	226	ALA	Peptide
1	B	65	GLY	Mainchain
1	B	95	PHE	Peptide
1	C	114	GLU	Peptide
1	C	251	ALA	Peptide
1	C	254	HIS	Peptide
1	C	263	LEU	Peptide
1	C	264	PRO	Peptide
1	C	62	VAL	Peptide
1	D	13	ALA	Peptide
2	E	114	SER	Peptide
2	E	115	MET	Peptide
2	E	116	ALA	Peptide
2	E	166	ASP	Peptide
3	F	123	THR	Mainchain
3	F	167	ARG	Peptide
3	F	168	ALA	Peptide
3	F	176	ARG	Peptide
3	F	208	ASN	Peptide
3	F	71	LEU	Peptide
3	F	97	ASP	Peptide
3	F	98	GLY	Peptide
2	M	187	ILE	Peptide
3	Q	1	MET	Peptide
3	Q	136	ARG	Peptide
3	Q	155	LEU	Mainchain
3	Q	171	GLY	Peptide
3	Q	2	SER	Peptide
3	Q	84	LEU	Peptide
3	Q	85	ILE	Peptide
3	Q	86	GLN	Peptide
3	Q	87	ILE	Peptide
3	Q	88	GLY	Peptide
3	Q	91	GLY	Peptide
3	Q	92	ILE	Peptide
3	Q	93	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1935	0	2015	522	4
1	B	1899	0	1989	442	2
1	C	1986	0	2074	329	0
1	D	1964	0	2055	298	0
2	E	1470	0	1540	190	0
2	M	1470	0	1540	154	0
3	F	1820	0	1951	392	4
3	Q	1815	0	1948	371	2
All	All	14359	0	15112	2509	8

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 85.

All (2509) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:HIS:CE1	1:B:57:PRO:HG3	1.26	1.70
2:E:61:PRO:HD3	3:F:178:TRP:CZ3	1.25	1.63
1:C:243:LEU:CD2	1:D:243:LEU:HD21	1.16	1.61
1:C:252:ARG:CB	1:C:257:LEU:HD23	1.16	1.61
1:B:10:LEU:CD1	1:B:21:LEU:CD2	1.80	1.59
3:F:84:LEU:CD2	3:F:94:LEU:HD23	1.32	1.57
1:C:231:ARG:HD3	1:C:249:LEU:CD2	1.35	1.56
1:B:10:LEU:HD11	1:B:21:LEU:CD2	1.34	1.56
1:B:24:LEU:HD11	1:B:218:VAL:CG1	1.35	1.55
1:B:247:LEU:HD11	1:B:249:LEU:CD2	1.13	1.55
1:C:252:ARG:C	1:C:257:LEU:HD21	1.26	1.55
1:C:252:ARG:HG2	1:C:257:LEU:CB	1.38	1.54
3:F:85:ILE:HG12	3:F:92:ILE:CG2	1.10	1.53
3:Q:65:TRP:CZ3	3:Q:117:LEU:HD12	1.36	1.52
1:B:24:LEU:CD1	1:B:218:VAL:HG13	1.37	1.52
1:A:24:LEU:CD1	1:A:218:VAL:HG23	1.34	1.51
1:C:231:ARG:CZ	1:C:249:LEU:HD21	1.38	1.50
1:C:263:LEU:HD22	1:C:264:PRO:CD	1.40	1.50
1:B:24:LEU:CD2	1:B:218:VAL:N	1.70	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:HIS:CE1	1:B:57:PRO:CG	1.91	1.50
3:Q:62:LEU:CB	3:Q:64:PHE:H	1.22	1.50
1:C:252:ARG:CG	1:C:257:LEU:HB3	1.42	1.48
3:F:132:LEU:CD2	3:F:137:VAL:HG21	1.40	1.47
3:Q:62:LEU:CA	3:Q:64:PHE:H	1.26	1.47
1:B:247:LEU:CD1	1:B:249:LEU:CD2	1.90	1.47
3:F:85:ILE:CG1	3:F:92:ILE:CG2	1.91	1.46
1:A:255:GLY:CA	1:A:257:LEU:HD11	1.45	1.46
1:A:208:ASP:C	1:A:224:ALA:HB2	1.37	1.45
3:Q:62:LEU:HB2	3:Q:64:PHE:N	1.28	1.45
1:A:255:GLY:C	1:A:257:LEU:CD1	1.87	1.45
1:C:252:ARG:O	1:C:257:LEU:CD2	1.64	1.45
3:F:97:ASP:O	3:F:99:PRO:CD	1.64	1.45
3:F:85:ILE:CG1	3:F:92:ILE:HG23	1.47	1.45
1:C:231:ARG:NE	1:C:249:LEU:HD21	1.28	1.44
1:A:24:LEU:HD11	1:A:218:VAL:CG2	1.48	1.42
1:A:99:VAL:CG2	1:A:136:ARG:O	1.63	1.42
1:B:24:LEU:HD21	1:B:218:VAL:N	1.25	1.41
1:C:243:LEU:CD2	1:D:243:LEU:CD2	1.99	1.41
3:Q:2:SER:HA	3:Q:3:ILE:CG2	1.48	1.41
1:B:24:LEU:CD1	1:B:218:VAL:CG1	1.93	1.41
1:C:73:ARG:NH2	1:C:80:ARG:NH1	1.62	1.40
1:A:125:LEU:CD2	1:A:130:ILE:HD11	1.48	1.40
1:A:255:GLY:C	1:A:257:LEU:HD11	1.45	1.40
3:Q:62:LEU:HB2	3:Q:64:PHE:CA	1.50	1.39
1:C:243:LEU:HD22	1:D:243:LEU:CD2	1.52	1.39
3:Q:162:MET:HE3	3:Q:192:ARG:NH1	1.36	1.38
1:C:231:ARG:CD	1:C:249:LEU:CD2	1.99	1.38
1:C:252:ARG:CG	1:C:257:LEU:HD23	1.51	1.38
1:A:252:ARG:HA	1:A:257:LEU:CG	1.44	1.38
3:Q:2:SER:CA	3:Q:3:ILE:HG23	1.54	1.38
1:C:252:ARG:C	1:C:257:LEU:CD2	1.94	1.36
2:M:60:ILE:HD12	3:Q:179:LEU:CD1	1.55	1.35
1:C:252:ARG:HG2	1:C:257:LEU:CD2	1.56	1.35
1:B:24:LEU:HD23	1:B:217:ARG:CA	1.57	1.35
1:C:16:GLY:O	3:F:8:ARG:NH1	1.57	1.35
1:A:125:LEU:HD22	1:A:130:ILE:CD1	1.56	1.34
1:A:259:PRO:O	1:A:265:LYS:HE2	1.19	1.33
3:Q:30:PHE:CE1	3:Q:234:GLN:HG2	1.61	1.33
1:B:247:LEU:CD1	1:B:249:LEU:HD22	1.55	1.33
3:Q:162:MET:CE	3:Q:192:ARG:NH1	1.90	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:GLU:OE1	1:C:134:ARG:NH1	1.63	1.31
1:B:50:HIS:ND1	1:B:57:PRO:HG3	1.44	1.30
1:C:252:ARG:HG2	1:C:257:LEU:CG	1.58	1.30
3:F:132:LEU:HD21	3:F:137:VAL:CG2	1.62	1.30
1:B:82:ARG:NH2	1:B:160:GLU:OE2	1.64	1.30
2:E:5:GLU:OE1	2:E:105:LEU:N	1.62	1.30
2:E:42:ARG:CD	3:F:211:GLY:O	1.80	1.29
3:F:84:LEU:CD2	3:F:94:LEU:CD2	2.10	1.29
2:E:61:PRO:CD	3:F:178:TRP:CZ3	2.16	1.28
1:C:252:ARG:CA	1:C:257:LEU:HD23	1.64	1.27
1:C:252:ARG:CG	1:C:257:LEU:CB	2.05	1.27
1:B:24:LEU:CG	1:B:218:VAL:HG13	1.64	1.27
1:C:17:GLY:O	1:C:18:VAL:HG22	1.33	1.27
2:E:58:LEU:O	2:E:69:HIS:NE2	1.67	1.27
1:A:255:GLY:O	1:A:257:LEU:CD1	1.78	1.26
1:B:50:HIS:CE1	1:B:57:PRO:CD	2.18	1.26
2:E:58:LEU:O	2:E:69:HIS:CD2	1.89	1.26
3:Q:61:PRO:O	3:Q:63:ARG:HB2	1.33	1.25
3:Q:65:TRP:CZ3	3:Q:117:LEU:CD1	2.18	1.25
1:C:252:ARG:CB	1:C:257:LEU:CD2	2.12	1.25
1:D:261:ALA:CB	1:D:262:PRO:HD3	1.67	1.24
1:A:114:GLU:CG	1:C:2:THR:HG21	1.65	1.24
1:B:10:LEU:CD1	1:B:21:LEU:HD23	1.47	1.24
1:C:256:LEU:CD2	1:C:258:ALA:HB2	1.66	1.23
3:F:236:ALA:O	3:F:237:ILE:O	1.56	1.23
1:C:252:ARG:CG	1:C:257:LEU:CD2	2.13	1.23
3:F:212:GLU:O	3:F:213:MET:HG2	1.36	1.23
1:B:73:ARG:O	1:B:74:LYS:NZ	1.70	1.23
1:B:10:LEU:O	1:B:59:SER:O	1.56	1.23
1:A:76:LEU:O	1:A:79:TRP:N	1.72	1.23
1:B:24:LEU:CG	1:B:218:VAL:CG1	2.13	1.23
1:B:224:ALA:O	1:B:228:LEU:HG	1.33	1.22
1:C:243:LEU:HD22	1:D:243:LEU:CG	1.68	1.22
3:Q:174:THR:OG1	3:Q:177:ARG:HG3	1.34	1.22
1:A:208:ASP:O	1:A:224:ALA:HB2	1.35	1.22
2:M:82:PRO:HD3	2:M:124:PHE:CE2	1.75	1.22
3:Q:66:ALA:O	3:Q:70:VAL:HG23	1.34	1.22
3:F:132:LEU:CD2	3:F:137:VAL:CG2	2.15	1.22
1:A:64:LEU:HD11	1:A:67:THR:OG1	1.41	1.21
1:A:109:ASN:ND2	3:Q:177:ARG:HH11	1.38	1.21
1:B:139:HIS:ND1	1:B:139:HIS:O	1.74	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ALA:HA	1:B:20:ALA:CB	1.71	1.20
1:D:261:ALA:HB3	1:D:262:PRO:CD	1.72	1.20
3:F:11:ALA:HB1	3:F:16:ARG:NH2	1.57	1.19
1:A:99:VAL:HG21	1:A:135:ASP:C	1.66	1.19
3:Q:62:LEU:CA	3:Q:64:PHE:N	2.05	1.19
1:C:224:ALA:O	1:C:228:LEU:HD12	1.40	1.19
3:F:209:TRP:HD1	3:F:210:GLN:O	1.23	1.18
1:D:101:GLU:C	1:D:104:SER:OG	1.86	1.18
3:Q:62:LEU:CB	3:Q:64:PHE:N	1.89	1.18
1:B:71:HIS:O	1:B:74:LYS:NZ	1.75	1.17
3:Q:65:TRP:CE3	3:Q:117:LEU:CD1	2.27	1.17
1:C:231:ARG:NE	1:C:249:LEU:CD2	2.06	1.17
3:Q:91:GLY:HA3	3:Q:92:ILE:HG23	1.21	1.16
3:Q:166:GLN:O	3:Q:168:ALA:O	1.63	1.16
3:Q:238:LEU:HD13	3:Q:239:ALA:N	1.60	1.16
1:A:56:ARG:HD2	1:A:57:PRO:N	1.60	1.16
1:B:247:LEU:CD1	1:B:249:LEU:HD23	1.58	1.16
1:C:61:ARG:NH2	1:C:63:LEU:HD11	1.61	1.16
3:F:97:ASP:C	3:F:99:PRO:CD	2.19	1.16
3:Q:238:LEU:CD1	3:Q:239:ALA:N	2.09	1.15
1:C:122:GLU:CD	1:C:134:ARG:HH12	1.55	1.15
3:F:84:LEU:HD23	3:F:94:LEU:CD2	1.74	1.15
3:Q:22:GLU:OE2	3:Q:226:VAL:CG2	1.94	1.15
3:F:84:LEU:HD21	3:F:94:LEU:CD2	1.73	1.15
1:A:112:LEU:HD12	1:A:116:GLU:HB2	1.21	1.15
1:B:50:HIS:HE1	1:B:57:PRO:N	1.44	1.15
2:E:60:ILE:HG22	2:E:61:PRO:O	1.45	1.15
1:A:128:LEU:O	1:A:182:LEU:CD1	1.95	1.14
1:A:255:GLY:H	1:A:257:LEU:HD21	1.10	1.14
1:B:60:GLY:O	1:B:61:ARG:HD2	1.45	1.14
1:A:24:LEU:HD12	1:A:218:VAL:N	1.63	1.14
2:E:61:PRO:HD3	3:F:178:TRP:CH2	1.83	1.14
3:F:242:VAL:HG13	3:F:243:LEU:HD22	1.23	1.14
1:B:10:LEU:HD13	1:B:21:LEU:CD2	1.60	1.13
3:Q:208:ASN:O	3:Q:209:TRP:HE3	1.28	1.13
3:F:98:GLY:N	3:F:99:PRO:HD3	1.58	1.13
3:Q:30:PHE:HE1	3:Q:234:GLN:CG	1.60	1.13
1:D:105:PHE:CE1	1:D:109:ASN:OD1	2.01	1.13
1:B:9:ALA:HB3	1:B:10:LEU:CA	1.79	1.12
1:B:70:GLY:O	1:B:75:ASP:HB3	1.49	1.12
3:Q:163:THR:HB	3:Q:167:ARG:HH22	1.08	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:174:THR:HG23	3:Q:177:ARG:CD	1.78	1.12
1:B:32:GLU:HG2	1:B:33:SER:N	1.57	1.12
1:A:139:HIS:CD2	1:A:146:LYS:NZ	2.17	1.12
1:A:223:ALA:HB3	1:A:226:ALA:HB3	1.12	1.12
1:D:243:LEU:HD23	1:D:244:VAL:N	1.64	1.12
1:A:230:ASP:CG	1:A:233:THR:OG1	1.93	1.12
1:C:251:ALA:O	1:C:254:HIS:O	1.67	1.12
3:Q:62:LEU:CB	3:Q:64:PHE:CA	2.27	1.12
1:C:13:ALA:O	1:C:14:PHE:HB2	1.49	1.12
1:C:263:LEU:CD2	1:C:264:PRO:CD	2.26	1.12
3:F:85:ILE:HD12	3:F:95:ALA:HA	1.26	1.12
1:B:24:LEU:HD23	1:B:217:ARG:C	1.75	1.11
1:B:96:ALA:CB	1:B:102:ASP:OD2	1.98	1.11
3:Q:65:TRP:CE3	3:Q:117:LEU:HD13	1.83	1.11
3:Q:174:THR:H	3:Q:177:ARG:HD3	1.14	1.11
1:A:134:ARG:N	1:A:135:ASP:HB2	1.66	1.11
1:B:24:LEU:HD23	1:B:217:ARG:HA	1.13	1.11
1:A:103:VAL:HG11	1:A:121:VAL:HG13	1.31	1.11
1:B:7:ALA:O	1:B:25:SER:HA	1.48	1.11
1:B:10:LEU:HD11	1:B:21:LEU:CG	1.78	1.11
1:B:70:GLY:N	1:B:75:ASP:OD2	1.84	1.11
1:D:105:PHE:HE1	1:D:109:ASN:OD1	1.33	1.11
2:E:104:GLY:HA3	2:E:107:THR:OG1	1.48	1.11
1:A:99:VAL:HG23	1:A:136:ARG:O	1.45	1.11
3:Q:162:MET:CE	3:Q:192:ARG:HH12	1.59	1.11
3:F:85:ILE:CD1	3:F:92:ILE:HG21	1.80	1.11
1:A:255:GLY:C	1:A:257:LEU:HD13	1.63	1.10
1:D:72:SER:N	1:D:73:ARG:HA	1.66	1.10
1:A:62:VAL:O	1:A:63:LEU:HG	1.49	1.10
1:A:230:ASP:CG	1:A:233:THR:HG1	1.56	1.10
1:A:252:ARG:HA	1:A:257:LEU:HG	1.13	1.10
1:B:9:ALA:HB3	1:B:10:LEU:HA	1.30	1.10
3:Q:174:THR:HG23	3:Q:177:ARG:HD2	1.30	1.10
1:C:252:ARG:CD	1:C:257:LEU:HB3	1.80	1.10
2:E:116:ALA:HB1	2:E:117:ILE:HA	1.27	1.10
3:F:24:SER:O	3:F:28:LEU:HD12	1.51	1.10
1:D:101:GLU:O	1:D:104:SER:OG	1.64	1.10
1:C:73:ARG:HG2	3:F:174:THR:HG23	1.16	1.09
1:C:231:ARG:CZ	1:C:249:LEU:CD2	2.30	1.09
1:C:263:LEU:CD2	1:C:264:PRO:HD2	1.82	1.09
3:F:212:GLU:C	3:F:213:MET:HG2	1.67	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ARG:HH21	1:C:63:LEU:CD1	1.64	1.09
1:C:173:LEU:HA	1:C:176:THR:HG22	1.29	1.09
1:A:223:ALA:HB3	1:A:226:ALA:CB	1.83	1.09
1:B:24:LEU:HD11	1:B:218:VAL:HG11	1.33	1.09
1:B:24:LEU:HG	1:B:218:VAL:HG12	1.22	1.09
1:B:32:GLU:OE2	1:B:209:ARG:HG3	1.52	1.09
2:E:42:ARG:NE	3:F:211:GLY:O	1.86	1.09
1:B:244:VAL:CG2	1:B:245:ILE:H	1.61	1.09
3:F:16:ARG:NH1	3:F:124:PRO:HG2	1.65	1.09
2:E:169:SER:HB2	3:F:86:GLN:HG3	1.20	1.08
3:F:209:TRP:CD1	3:F:210:GLN:O	2.06	1.08
3:Q:223:SER:HB3	3:Q:225:ARG:HG2	1.24	1.08
1:A:139:HIS:CD2	1:A:146:LYS:HZ3	1.71	1.08
1:B:61:ARG:NH2	1:B:71:HIS:HE1	1.51	1.08
1:A:10:LEU:HG	1:A:10:LEU:O	1.50	1.07
1:B:71:HIS:O	1:B:73:ARG:N	1.87	1.07
1:D:96:ALA:HB3	1:D:102:ASP:CB	1.83	1.07
1:A:97:THR:HA	1:A:138:THR:OG1	1.53	1.07
1:A:99:VAL:HG22	1:A:136:ARG:O	1.24	1.07
3:Q:201:GLU:HG3	3:Q:210:GLN:HG3	1.35	1.07
3:F:212:GLU:O	3:F:213:MET:CG	2.03	1.07
1:A:112:LEU:CD1	1:A:116:GLU:HB2	1.85	1.06
1:A:259:PRO:O	1:A:265:LYS:CE	2.02	1.06
2:E:112:ALA:O	2:E:116:ALA:O	1.73	1.06
3:F:16:ARG:HH11	3:F:124:PRO:CG	1.67	1.06
1:A:134:ARG:HA	1:A:135:ASP:O	1.54	1.06
1:B:21:LEU:O	1:B:22:ASP:O	1.73	1.06
1:B:32:GLU:HG2	1:B:33:SER:H	0.93	1.06
1:C:120:ARG:HH12	1:C:158:ARG:HD2	1.16	1.06
1:C:252:ARG:HB3	1:C:257:LEU:HD23	1.30	1.06
2:E:104:GLY:CA	2:E:107:THR:OG1	2.03	1.05
1:A:114:GLU:HG3	1:C:2:THR:CG2	1.86	1.05
1:B:221:GLU:O	1:B:221:GLU:CD	2.00	1.05
1:C:243:LEU:HD22	1:D:243:LEU:CD1	1.85	1.05
2:E:169:SER:CB	3:F:86:GLN:HG3	1.86	1.05
1:B:238:ALA:O	1:B:239:LEU:HD13	1.57	1.05
3:Q:174:THR:OG1	3:Q:177:ARG:CG	2.04	1.05
1:C:61:ARG:HH21	1:C:63:LEU:HD11	1.08	1.05
1:C:122:GLU:OE1	1:C:134:ARG:CZ	2.03	1.05
1:A:10:LEU:HD22	1:A:21:LEU:HG	1.38	1.04
1:A:255:GLY:O	1:A:257:LEU:HD13	1.47	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:85:ILE:CD1	3:F:92:ILE:CG2	2.34	1.04
1:A:255:GLY:HA3	1:A:257:LEU:HD11	1.07	1.04
1:D:256:LEU:HG	1:D:257:LEU:HD23	1.06	1.04
2:M:60:ILE:HD12	3:Q:179:LEU:HD12	1.39	1.04
2:M:166:ASP:OD2	2:M:169:SER:N	1.90	1.04
1:A:208:ASP:HA	1:A:224:ALA:CB	1.88	1.03
1:A:249:LEU:HD23	1:A:249:LEU:H	1.20	1.03
1:B:60:GLY:O	1:B:61:ARG:CD	2.05	1.03
3:F:139:ALA:O	3:F:142:ILE:CD1	2.06	1.03
1:B:50:HIS:ND1	1:B:57:PRO:CG	2.10	1.03
3:Q:85:ILE:HB	3:Q:86:GLN:HB3	1.36	1.02
1:C:263:LEU:HD22	1:C:264:PRO:HD2	1.34	1.02
1:A:114:GLU:OE2	1:A:114:GLU:N	1.93	1.02
1:A:132:ASP:HB3	1:A:133:LEU:HA	1.39	1.02
1:A:208:ASP:CA	1:A:224:ALA:HB2	1.88	1.02
1:A:269:ALA:HB1	1:A:270:LEU:HB2	1.42	1.02
1:D:261:ALA:HB3	1:D:262:PRO:HD3	1.29	1.02
1:B:8:GLU:HA	1:B:25:SER:HB3	1.41	1.02
1:C:231:ARG:HD3	1:C:249:LEU:HD23	1.04	1.02
3:F:85:ILE:CG1	3:F:92:ILE:HG21	1.79	1.02
1:B:32:GLU:HG3	1:B:208:ASP:HB2	1.42	1.02
1:B:244:VAL:HG22	1:B:245:ILE:N	1.61	1.02
1:C:17:GLY:O	1:C:18:VAL:CG2	2.08	1.02
1:A:252:ARG:CA	1:A:257:LEU:CG	2.38	1.01
1:A:255:GLY:N	1:A:257:LEU:HD21	1.75	1.01
3:Q:30:PHE:HE1	3:Q:234:GLN:HG2	0.87	1.01
1:C:113:SER:OG	1:C:115:ALA:HB3	1.60	1.01
1:A:208:ASP:C	1:A:224:ALA:CB	2.33	1.01
1:C:231:ARG:HD3	1:C:249:LEU:HD22	1.40	1.01
3:Q:65:TRP:CE3	3:Q:117:LEU:HD12	1.94	1.01
3:F:45:LEU:H	3:F:45:LEU:HD12	1.26	1.01
1:B:10:LEU:HD11	1:B:21:LEU:HD21	1.04	1.01
3:Q:66:ALA:O	3:Q:70:VAL:CG2	2.07	1.01
1:B:7:ALA:O	1:B:25:SER:CA	2.09	1.01
1:B:13:ALA:HA	1:B:20:ALA:HB2	1.41	1.01
1:C:256:LEU:HD22	1:C:258:ALA:HB2	1.40	1.01
1:D:96:ALA:HB3	1:D:102:ASP:HB2	1.42	1.01
3:F:85:ILE:HG12	3:F:92:ILE:HG22	1.39	1.01
3:F:85:ILE:HD12	3:F:95:ALA:CA	1.89	1.01
3:F:22:GLU:OE2	3:F:222:ALA:CB	2.08	1.00
1:A:255:GLY:HA3	1:A:257:LEU:CD1	1.91	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:ALA:CB	1:D:102:ASP:HA	1.91	1.00
1:B:9:ALA:HB3	1:B:10:LEU:C	1.86	1.00
1:A:263:LEU:H	1:A:263:LEU:HD12	1.22	1.00
2:M:166:ASP:HB2	2:M:173:GLY:HA3	1.40	1.00
1:D:230:ASP:OD1	1:D:233:THR:N	1.93	0.99
2:M:61:PRO:HD2	3:Q:179:LEU:HD13	1.44	0.99
1:C:19:LYS:O	1:C:19:LYS:HG2	1.58	0.99
1:C:122:GLU:OE1	1:C:134:ARG:NH2	1.96	0.99
3:Q:86:GLN:HG3	3:Q:87:ILE:HG13	1.44	0.99
3:F:47:THR:O	3:F:50:ILE:HG22	1.61	0.99
2:M:60:ILE:CD1	3:Q:179:LEU:HD12	1.93	0.99
1:D:256:LEU:CG	1:D:257:LEU:HD23	1.92	0.99
1:C:113:SER:OG	1:C:115:ALA:CB	2.11	0.98
3:F:97:ASP:O	3:F:99:PRO:HD2	0.83	0.98
3:Q:22:GLU:OE2	3:Q:226:VAL:HG21	1.59	0.98
3:Q:162:MET:CE	3:Q:192:ARG:CZ	2.41	0.98
2:M:60:ILE:CD1	3:Q:179:LEU:CD1	2.41	0.98
3:Q:238:LEU:CD1	3:Q:239:ALA:H	1.70	0.98
1:C:243:LEU:HD22	1:D:243:LEU:HD21	1.05	0.98
3:F:16:ARG:HH11	3:F:124:PRO:HG2	0.84	0.98
1:B:118:ARG:HB3	1:B:118:ARG:HH11	1.29	0.98
3:F:166:GLN:O	3:F:168:ALA:O	1.80	0.98
1:D:74:LYS:HA	1:D:77:THR:OG1	1.62	0.98
3:F:39:PRO:C	3:F:41:PRO:HA	1.88	0.98
1:A:76:LEU:HD13	1:A:80:ARG:HG2	1.43	0.98
1:B:247:LEU:HD11	1:B:249:LEU:HD22	1.18	0.98
1:D:17:GLY:O	1:D:18:VAL:HG12	1.65	0.97
1:C:252:ARG:O	1:C:257:LEU:HD21	0.81	0.97
1:A:99:VAL:CG2	1:A:135:ASP:C	2.38	0.97
1:B:96:ALA:HB1	1:B:102:ASP:OD2	1.64	0.97
1:B:26:LEU:HD12	1:B:27:ALA:N	1.79	0.97
1:A:259:PRO:HD2	1:A:265:LYS:CE	1.95	0.97
1:A:173:LEU:O	1:A:177:GLU:OE1	1.81	0.97
1:A:252:ARG:CA	1:A:257:LEU:HG	1.94	0.97
2:M:100:LEU:CD2	3:Q:3:ILE:HG21	1.94	0.97
1:D:71:HIS:CE1	1:D:73:ARG:HG3	1.99	0.97
3:Q:62:LEU:HA	3:Q:63:ARG:CB	1.95	0.97
3:Q:162:MET:HE1	3:Q:192:ARG:CZ	1.94	0.97
1:B:204:ALA:O	1:B:261:ALA:HB1	1.62	0.97
1:C:263:LEU:CD2	1:C:264:PRO:HD3	1.89	0.97
1:A:24:LEU:HD12	1:A:218:VAL:H	1.21	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:62:LEU:HA	3:Q:64:PHE:N	1.76	0.97
3:Q:177:ARG:O	3:Q:181:SER:OG	1.81	0.97
1:D:260:GLU:N	1:D:260:GLU:OE2	1.97	0.97
3:F:98:GLY:N	3:F:99:PRO:CD	2.28	0.97
3:Q:208:ASN:O	3:Q:209:TRP:CE3	2.15	0.96
1:C:73:ARG:O	1:C:74:LYS:C	2.07	0.96
1:B:24:LEU:CD2	1:B:218:VAL:HG13	1.94	0.96
3:Q:223:SER:HB3	3:Q:225:ARG:CG	1.95	0.96
1:A:247:LEU:HA	1:A:250:LEU:HD12	1.48	0.96
3:Q:65:TRP:O	3:Q:68:VAL:N	1.99	0.96
1:B:13:ALA:CA	1:B:20:ALA:CB	2.43	0.96
1:B:204:ALA:O	1:B:261:ALA:CB	2.14	0.96
1:C:252:ARG:CA	1:C:257:LEU:CD2	2.30	0.96
1:D:96:ALA:HB2	1:D:102:ASP:HA	1.47	0.96
2:E:61:PRO:HD3	3:F:178:TRP:CE3	2.00	0.96
3:Q:61:PRO:O	3:Q:63:ARG:CB	2.15	0.95
1:A:15:PRO:C	1:A:17:GLY:HA2	1.92	0.95
1:A:208:ASP:O	1:A:224:ALA:CB	2.15	0.95
1:B:50:HIS:CE1	1:B:57:PRO:N	2.32	0.95
1:B:74:LYS:O	1:B:77:THR:OG1	1.85	0.95
3:Q:130:SER:OG	3:Q:219:ARG:NH1	2.00	0.95
3:Q:238:LEU:HD12	3:Q:239:ALA:H	1.30	0.95
3:Q:163:THR:HB	3:Q:167:ARG:NH2	1.80	0.95
1:A:15:PRO:HG3	3:Q:8:ARG:HD3	1.48	0.94
3:Q:174:THR:HG1	3:Q:177:ARG:HG3	1.22	0.94
1:A:100:PHE:O	1:A:104:SER:OG	1.85	0.94
1:D:109:ASN:HD22	1:D:109:ASN:H	1.02	0.94
3:F:30:PHE:HE1	3:F:234:GLN:HG2	1.33	0.94
1:B:120:ARG:HH21	1:B:158:ARG:CZ	1.81	0.94
1:B:221:GLU:O	1:B:221:GLU:CG	2.11	0.94
3:Q:91:GLY:CA	3:Q:92:ILE:HG23	1.97	0.94
3:Q:168:ALA:C	3:Q:170:LEU:H	1.71	0.94
3:F:78:THR:O	3:F:82:VAL:HG13	1.68	0.94
1:B:32:GLU:CG	1:B:208:ASP:HB2	1.98	0.94
1:D:71:HIS:CE1	1:D:73:ARG:HH21	1.84	0.94
1:D:249:LEU:O	1:D:251:ALA:N	2.01	0.94
1:D:261:ALA:HB1	1:D:262:PRO:HD3	1.50	0.94
1:B:24:LEU:HD23	1:B:218:VAL:N	1.57	0.94
1:A:14:PHE:HB3	1:A:18:VAL:CG2	1.97	0.94
1:B:10:LEU:CD1	1:B:21:LEU:HD21	1.63	0.94
1:C:243:LEU:HD21	1:D:243:LEU:HD21	0.95	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:97:ASP:C	3:F:99:PRO:HD2	1.84	0.93
3:Q:66:ALA:HA	3:Q:69:ALA:HB3	1.49	0.93
1:C:243:LEU:HD22	1:D:243:LEU:HD11	1.49	0.93
1:C:243:LEU:HD21	1:D:243:LEU:CD2	1.78	0.93
2:E:8:LEU:HD12	2:E:9:PRO:HD2	1.50	0.93
3:F:204:LEU:O	3:F:208:ASN:O	1.84	0.93
3:F:85:ILE:HD11	3:F:92:ILE:HG21	1.45	0.93
1:A:10:LEU:HD22	1:A:21:LEU:CG	1.76	0.93
1:A:114:GLU:HG3	1:C:2:THR:HG21	0.94	0.93
1:B:244:VAL:HG22	1:B:245:ILE:H	0.77	0.93
1:A:10:LEU:HD23	1:A:24:LEU:HB3	1.49	0.93
2:E:41:ALA:O	2:E:44:THR:OG1	1.85	0.93
1:A:97:THR:O	1:A:138:THR:N	2.01	0.93
1:C:263:LEU:HD22	1:C:264:PRO:HD3	0.94	0.93
2:E:42:ARG:HD3	3:F:211:GLY:O	1.68	0.93
3:F:236:ALA:O	3:F:237:ILE:C	2.09	0.93
1:C:231:ARG:HH12	1:C:250:LEU:HD21	1.33	0.92
1:D:76:LEU:O	1:D:80:ARG:CG	2.18	0.92
3:F:237:ILE:O	3:F:240:ALA:N	2.02	0.92
1:A:255:GLY:CA	1:A:257:LEU:CD1	2.32	0.92
1:A:147:ARG:NH1	1:A:166:GLU:O	2.02	0.92
1:C:73:ARG:HG2	3:F:174:THR:CG2	1.99	0.92
1:C:19:LYS:O	1:C:19:LYS:CG	2.13	0.92
1:D:101:GLU:CA	1:D:104:SER:OG	2.18	0.92
1:B:139:HIS:O	1:B:139:HIS:CG	2.22	0.92
1:A:109:ASN:ND2	3:Q:177:ARG:NH1	2.16	0.92
1:C:12:TYR:OH	1:C:14:PHE:CE1	2.23	0.92
2:M:82:PRO:HD3	2:M:124:PHE:CZ	2.03	0.92
3:F:177:ARG:HB3	3:F:180:ARG:HD2	1.51	0.91
1:A:103:VAL:CG1	1:A:121:VAL:HG13	2.01	0.91
1:B:24:LEU:HG	1:B:218:VAL:CG1	1.86	0.91
1:A:62:VAL:O	1:A:63:LEU:CG	2.18	0.91
1:A:83:VAL:HG22	1:A:161:VAL:HB	1.52	0.91
3:Q:62:LEU:HB2	3:Q:65:TRP:N	1.84	0.91
1:C:112:LEU:HB3	1:C:116:GLU:HB3	1.52	0.91
1:C:252:ARG:NE	1:C:257:LEU:HB3	1.85	0.91
2:M:82:PRO:CD	2:M:124:PHE:CE2	2.54	0.91
1:B:69:THR:HB	1:B:75:ASP:OD2	1.70	0.91
1:B:73:ARG:O	1:B:74:LYS:CD	2.18	0.91
3:F:177:ARG:HB3	3:F:180:ARG:HB2	1.50	0.91
1:A:76:LEU:C	1:A:76:LEU:HD12	1.95	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:HB2	1:A:79:TRP:HB3	1.51	0.91
1:A:103:VAL:HG12	1:A:121:VAL:HG22	1.53	0.91
1:D:96:ALA:CB	1:D:102:ASP:CA	2.49	0.91
1:D:109:ASN:HD22	1:D:109:ASN:N	1.68	0.91
3:Q:65:TRP:HZ3	3:Q:117:LEU:HD12	1.30	0.90
3:F:158:GLU:OE1	3:F:192:ARG:NH2	2.03	0.90
1:B:26:LEU:HD21	1:B:34:LEU:HD21	1.52	0.90
3:F:42:GLY:O	3:F:45:LEU:HD12	1.70	0.90
1:C:249:LEU:HG	1:C:250:LEU:CD2	2.01	0.90
1:A:64:LEU:HD11	1:A:67:THR:HG1	1.35	0.90
1:A:112:LEU:HD12	1:A:116:GLU:CB	2.00	0.90
2:M:62:SER:OG	2:M:188:PRO:HB3	1.71	0.90
1:D:76:LEU:O	1:D:80:ARG:HG2	1.69	0.90
3:Q:238:LEU:O	3:Q:241:GLY:N	2.04	0.90
1:A:13:ALA:HB1	1:A:19:LYS:H	1.34	0.90
3:F:42:GLY:HA2	3:F:45:LEU:CD1	2.02	0.90
1:B:8:GLU:CA	1:B:25:SER:HB3	2.02	0.90
3:Q:62:LEU:HB2	3:Q:64:PHE:C	1.96	0.90
3:Q:143:GLU:CD	3:Q:212:GLU:O	2.15	0.90
3:F:22:GLU:OE2	3:F:222:ALA:HB1	1.70	0.90
1:A:252:ARG:HA	1:A:257:LEU:CB	2.00	0.89
1:B:10:LEU:O	1:B:11:THR:OG1	1.87	0.89
1:B:60:GLY:C	1:B:61:ARG:HD2	1.96	0.89
1:B:224:ALA:O	1:B:228:LEU:CG	2.20	0.89
3:Q:85:ILE:HD12	3:Q:86:GLN:NE2	1.87	0.89
1:B:9:ALA:CB	1:B:10:LEU:CA	2.47	0.89
1:B:265:LYS:HD2	1:B:267:ARG:N	1.86	0.89
3:F:139:ALA:O	3:F:142:ILE:HD12	1.69	0.89
1:A:132:ASP:CA	1:A:134:ARG:HB2	2.03	0.89
1:A:185:GLY:O	1:A:188:ALA:HB3	1.73	0.89
1:B:24:LEU:CD2	1:B:217:ARG:HA	2.01	0.89
1:B:32:GLU:CG	1:B:33:SER:H	1.83	0.89
1:A:269:ALA:HB1	1:A:270:LEU:CB	2.02	0.89
2:M:164:TYR:O	2:M:165:PRO:O	1.89	0.89
3:Q:15:TRP:H	3:Q:16:ARG:NH2	1.70	0.89
1:B:247:LEU:HD12	1:B:249:LEU:HB2	1.53	0.89
2:M:60:ILE:HD12	3:Q:179:LEU:HD11	1.54	0.89
3:F:92:ILE:HG13	3:F:93:GLY:H	1.38	0.88
1:A:97:THR:O	1:A:138:THR:OG1	1.90	0.88
1:A:132:ASP:HA	1:A:134:ARG:HB2	1.56	0.88
3:F:177:ARG:O	3:F:180:ARG:CB	2.22	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:O	1:A:151:ILE:HG13	1.74	0.88
1:B:74:LYS:HG2	1:B:75:ASP:H	1.38	0.88
1:D:71:HIS:HE1	1:D:73:ARG:HH21	1.17	0.88
1:B:61:ARG:NH2	1:B:71:HIS:CE1	2.42	0.88
1:B:120:ARG:HH21	1:B:158:ARG:NE	1.71	0.88
1:B:70:GLY:O	1:B:74:LYS:NZ	2.06	0.88
1:B:224:ALA:HB1	1:B:228:LEU:HD23	1.54	0.88
1:B:13:ALA:CA	1:B:20:ALA:HB3	2.03	0.88
1:C:231:ARG:NH1	1:C:249:LEU:HD21	1.88	0.88
2:E:41:ALA:O	2:E:45:LEU:HD12	1.74	0.88
1:B:9:ALA:CB	1:B:10:LEU:C	2.46	0.87
1:C:73:ARG:CZ	1:C:76:LEU:HD13	2.04	0.87
1:C:58:GLN:OE1	1:C:58:GLN:N	2.07	0.87
3:Q:22:GLU:OE2	3:Q:226:VAL:HG23	1.72	0.87
3:Q:82:VAL:HA	3:Q:85:ILE:HD11	1.57	0.87
3:Q:82:VAL:O	3:Q:85:ILE:HG12	1.72	0.87
1:B:32:GLU:CD	1:B:209:ARG:HG3	1.99	0.87
1:D:95:PHE:HE2	3:F:213:MET:HB2	1.40	0.87
1:A:8:GLU:HB3	1:A:61:ARG:HB3	1.55	0.87
1:B:60:GLY:O	1:B:61:ARG:NE	2.06	0.87
3:Q:235:ALA:O	3:Q:238:LEU:HB3	1.75	0.87
1:A:208:ASP:CA	1:A:224:ALA:CB	2.48	0.87
1:C:15:PRO:O	3:F:8:ARG:HG2	1.75	0.87
1:B:24:LEU:HD21	1:B:218:VAL:CA	2.03	0.86
3:Q:228:GLY:O	3:Q:232:THR:HG23	1.75	0.86
1:C:224:ALA:O	1:C:228:LEU:CD1	2.22	0.86
1:D:101:GLU:HA	1:D:104:SER:OG	1.75	0.86
3:F:93:GLY:O	3:F:94:LEU:HB2	1.75	0.86
3:F:22:GLU:OE2	3:F:222:ALA:HB2	1.75	0.86
3:F:177:ARG:O	3:F:180:ARG:HB3	1.75	0.86
1:B:50:HIS:NE2	1:B:57:PRO:HG3	1.88	0.86
3:F:16:ARG:NH1	3:F:124:PRO:CG	2.32	0.86
1:B:234:LEU:HD13	1:B:235:ALA:CA	2.05	0.86
1:A:223:ALA:CB	1:A:226:ALA:CB	2.53	0.86
1:C:231:ARG:NH1	1:C:249:LEU:CD2	2.39	0.86
1:D:63:LEU:HD12	1:D:67:THR:O	1.75	0.86
3:F:97:ASP:C	3:F:99:PRO:HD3	1.94	0.86
3:Q:163:THR:HG22	3:Q:167:ARG:HH12	1.38	0.86
1:C:72:SER:O	1:C:76:LEU:HB2	1.74	0.86
1:A:132:ASP:C	1:A:134:ARG:HB2	2.01	0.86
1:B:10:LEU:HD13	1:B:21:LEU:HD23	0.86	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:LEU:CD2	1:D:243:LEU:CG	2.46	0.85
1:A:132:ASP:HB3	1:A:133:LEU:CA	2.05	0.85
1:C:173:LEU:HA	1:C:176:THR:CG2	2.05	0.85
3:F:85:ILE:HG12	3:F:92:ILE:HG21	1.41	0.85
1:A:15:PRO:HD2	1:A:18:VAL:HG13	1.58	0.85
1:D:105:PHE:HE1	1:D:109:ASN:CG	1.83	0.85
1:B:62:VAL:CG1	1:B:79:TRP:CZ2	2.58	0.85
1:B:13:ALA:HA	1:B:20:ALA:HB3	1.58	0.85
3:Q:174:THR:N	3:Q:177:ARG:HD3	1.92	0.85
1:D:244:VAL:HG21	1:D:261:ALA:O	1.75	0.85
1:B:32:GLU:HG3	1:B:208:ASP:CB	2.06	0.85
1:A:102:ASP:O	3:Q:169:ARG:NH1	2.09	0.85
1:A:256:LEU:C	1:A:257:LEU:HD13	2.01	0.85
2:E:58:LEU:C	2:E:69:HIS:NE2	2.29	0.85
1:C:231:ARG:NH1	1:C:250:LEU:HD21	1.92	0.85
3:F:31:LEU:O	3:F:35:VAL:HG23	1.77	0.85
1:A:147:ARG:HH22	1:A:169:ALA:HB3	1.41	0.85
1:C:256:LEU:CD2	1:C:258:ALA:CB	2.52	0.84
1:A:15:PRO:CD	1:A:18:VAL:HG22	2.07	0.84
1:A:129:SER:HB3	1:A:182:LEU:HD11	1.57	0.84
1:B:24:LEU:HD11	1:B:218:VAL:HG13	0.90	0.84
1:D:105:PHE:CD1	1:D:109:ASN:ND2	2.45	0.84
3:F:22:GLU:CG	3:F:222:ALA:CB	2.56	0.84
1:A:113:SER:O	1:A:115:ALA:N	2.10	0.84
1:C:120:ARG:HH11	1:C:120:ARG:HG2	1.43	0.84
1:C:252:ARG:O	1:C:257:LEU:CG	2.25	0.84
2:E:116:ALA:CB	2:E:117:ILE:HA	2.08	0.84
1:C:256:LEU:HD23	1:C:258:ALA:N	1.92	0.84
1:D:71:HIS:N	1:D:75:ASP:OD2	2.11	0.84
1:D:105:PHE:HD1	1:D:109:ASN:HD21	1.21	0.84
1:B:74:LYS:HG2	1:B:75:ASP:N	1.93	0.84
2:M:82:PRO:HG3	2:M:124:PHE:CE1	2.13	0.84
3:F:11:ALA:CB	3:F:16:ARG:NH2	2.39	0.84
1:B:247:LEU:HD12	1:B:249:LEU:CD2	2.06	0.84
1:B:234:LEU:HD13	1:B:235:ALA:N	1.93	0.84
1:D:105:PHE:CE1	1:D:109:ASN:CG	2.56	0.84
1:B:10:LEU:CD1	1:B:21:LEU:CG	2.47	0.83
1:B:50:HIS:CG	1:B:57:PRO:HG3	2.13	0.83
1:C:173:LEU:CA	1:C:176:THR:HG22	2.06	0.83
3:F:11:ALA:CB	3:F:16:ARG:CZ	2.56	0.83
1:A:95:PHE:CE2	3:Q:166:GLN:HG3	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:37:VAL:CG1	3:Q:42:GLY:HA3	2.08	0.83
1:A:10:LEU:HD11	1:A:21:LEU:C	2.03	0.83
3:Q:168:ALA:O	3:Q:170:LEU:N	2.11	0.83
1:C:30:LYS:O	1:C:192:THR:OG1	1.95	0.83
1:C:73:ARG:HH21	1:C:80:ARG:NH1	1.69	0.83
1:A:15:PRO:CD	1:A:18:VAL:HG13	2.08	0.83
2:M:100:LEU:HD21	3:Q:3:ILE:HG21	1.58	0.83
3:F:50:ILE:O	3:F:54:THR:HG23	1.78	0.83
1:B:50:HIS:CE1	1:B:57:PRO:HD3	2.12	0.83
1:B:96:ALA:HB2	1:B:102:ASP:OD2	1.78	0.83
3:F:30:PHE:CE1	3:F:234:GLN:HG2	2.13	0.83
3:F:172:HIS:CD2	3:F:178:TRP:CD1	2.66	0.83
1:A:139:HIS:HD2	1:A:146:LYS:CE	1.90	0.83
1:B:234:LEU:HD13	1:B:235:ALA:HA	1.60	0.83
1:D:110:LEU:HD11	1:D:157:MET:HB3	1.61	0.83
1:A:144:GLY:O	1:A:147:ARG:N	2.11	0.83
1:A:257:LEU:H	1:A:257:LEU:HD22	1.44	0.83
1:B:73:ARG:O	1:B:74:LYS:CE	2.25	0.83
1:B:114:GLU:O	1:B:118:ARG:HG3	1.79	0.83
1:D:13:ALA:HB2	1:D:19:LYS:HA	1.61	0.83
1:D:98:THR:HG22	1:D:101:GLU:OE2	1.78	0.83
1:D:261:ALA:HB3	1:D:262:PRO:HD2	1.60	0.82
1:D:14:PHE:CE2	1:D:15:PRO:HB3	2.14	0.82
3:F:212:GLU:C	3:F:213:MET:CG	2.48	0.82
1:A:244:VAL:HG13	1:A:245:ILE:N	1.94	0.82
2:M:59:LYS:HG3	2:M:69:HIS:HD2	1.42	0.82
3:Q:163:THR:CG2	3:Q:167:ARG:HH12	1.91	0.82
1:A:132:ASP:CB	1:A:133:LEU:HA	2.08	0.82
1:C:73:ARG:NH2	1:C:80:ARG:HH11	1.72	0.82
1:D:256:LEU:HG	1:D:257:LEU:CD2	2.01	0.82
3:F:50:ILE:HG23	3:F:51:LEU:CD2	2.09	0.82
1:A:97:THR:CA	1:A:138:THR:OG1	2.27	0.82
3:Q:82:VAL:O	3:Q:85:ILE:CG1	2.28	0.82
1:A:95:PHE:CZ	3:Q:166:GLN:HG3	2.14	0.82
1:A:147:ARG:NH1	1:A:167:PRO:C	2.37	0.82
2:E:4:MET:O	2:E:107:THR:HG21	1.80	0.82
1:C:231:ARG:CD	1:C:249:LEU:HD23	1.85	0.82
1:A:152:ALA:O	1:A:155:VAL:HG22	1.79	0.81
1:A:247:LEU:O	1:A:251:ALA:N	2.13	0.81
3:Q:15:TRP:H	3:Q:16:ARG:HH21	1.23	0.81
1:C:15:PRO:O	3:F:8:ARG:CG	2.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:42:ARG:HD2	3:F:211:GLY:O	1.78	0.81
1:A:10:LEU:HD11	1:A:21:LEU:O	1.80	0.81
1:A:178:GLN:OE1	1:A:178:GLN:N	2.14	0.81
1:B:13:ALA:N	1:B:20:ALA:HB3	1.96	0.81
3:Q:19:PRO:HB2	3:Q:222:ALA:HB2	1.62	0.81
1:C:111:GLY:O	1:C:113:SER:N	2.12	0.81
1:A:249:LEU:HG	1:A:250:LEU:H	1.45	0.81
3:F:132:LEU:HD23	3:F:137:VAL:CG2	2.11	0.81
1:B:10:LEU:HD11	1:B:21:LEU:HG	1.62	0.81
1:B:13:ALA:CA	1:B:20:ALA:HB2	2.06	0.81
1:D:71:HIS:CE1	1:D:73:ARG:CG	2.63	0.81
3:Q:174:THR:HG23	3:Q:177:ARG:HD3	1.62	0.81
2:E:174:ALA:HA	2:E:177:LYS:HE2	1.63	0.81
1:B:73:ARG:HA	1:B:76:LEU:HD11	1.62	0.81
1:B:234:LEU:O	1:B:234:LEU:HD22	1.79	0.81
3:Q:143:GLU:OE1	3:Q:212:GLU:O	1.98	0.81
3:Q:174:THR:CG2	3:Q:177:ARG:CD	2.58	0.81
1:A:15:PRO:HD3	1:A:18:VAL:HG22	1.63	0.81
1:A:122:GLU:HG3	1:A:123:GLU:N	1.94	0.81
3:Q:22:GLU:CD	3:Q:222:ALA:HB1	2.06	0.81
1:B:50:HIS:HE1	1:B:57:PRO:CD	1.71	0.80
1:B:242:PRO:O	1:B:244:VAL:HG12	1.81	0.80
1:D:105:PHE:O	1:D:109:ASN:ND2	2.14	0.80
1:B:24:LEU:CD2	1:B:217:ARG:CA	2.51	0.80
3:Q:86:GLN:C	3:Q:87:ILE:HG13	2.06	0.80
1:C:252:ARG:CG	1:C:257:LEU:CG	2.34	0.80
3:F:47:THR:O	3:F:51:LEU:HD23	1.82	0.80
1:A:135:ASP:HA	1:A:136:ARG:C	2.05	0.80
1:B:6:ALA:O	1:B:63:LEU:HD22	1.81	0.80
1:B:139:HIS:CD2	3:Q:153:PHE:HB3	2.16	0.80
1:C:252:ARG:HG2	1:C:257:LEU:HB3	0.94	0.80
1:A:114:GLU:H	1:A:114:GLU:CD	1.86	0.80
1:A:223:ALA:CB	1:A:226:ALA:HB3	2.03	0.80
1:B:12:TYR:C	1:B:20:ALA:HB3	2.06	0.80
1:A:10:LEU:O	1:A:10:LEU:CG	2.29	0.80
1:B:11:THR:CB	1:B:59:SER:O	2.30	0.80
3:Q:62:LEU:CA	3:Q:63:ARG:HB2	2.12	0.80
1:C:248:ALA:O	1:C:252:ARG:HB2	1.80	0.80
1:C:114:GLU:N	1:C:115:ALA:HB3	1.95	0.80
1:D:162:LEU:HD23	1:D:164:LEU:HD11	1.63	0.80
1:A:99:VAL:HG21	1:A:136:ARG:N	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:HD12	1:A:111:GLY:H	1.46	0.80
1:B:62:VAL:HG11	1:B:79:TRP:CZ2	2.16	0.80
1:A:145:GLN:OE1	1:A:148:ARG:NH1	2.14	0.80
1:B:73:ARG:O	1:B:74:LYS:CG	2.30	0.80
3:Q:201:GLU:HG3	3:Q:210:GLN:CG	2.12	0.80
1:B:24:LEU:CD1	1:B:218:VAL:HG11	1.98	0.80
1:C:249:LEU:HG	1:C:250:LEU:HD23	1.64	0.80
1:C:256:LEU:HD21	1:C:258:ALA:HB2	1.64	0.80
2:E:108:LEU:HD23	2:E:109:GLY:N	1.97	0.80
1:A:24:LEU:CG	1:A:218:VAL:HG23	2.11	0.80
1:B:62:VAL:HG11	1:B:79:TRP:HZ2	1.47	0.80
2:M:82:PRO:CD	2:M:124:PHE:CZ	2.64	0.80
1:D:37:LEU:HD12	1:D:38:GLY:H	1.45	0.79
1:B:71:HIS:H	1:B:71:HIS:CD2	1.96	0.79
3:F:165:ALA:O	3:F:168:ALA:O	2.00	0.79
1:D:262:PRO:O	1:D:264:PRO:HD3	1.83	0.79
3:Q:19:PRO:HG3	3:Q:220:PRO:HG2	1.65	0.79
3:Q:22:GLU:OE2	3:Q:222:ALA:HB1	1.83	0.79
1:A:14:PHE:H	1:A:18:VAL:CG2	1.96	0.79
3:F:85:ILE:HG12	3:F:92:ILE:HG23	0.80	0.79
1:A:14:PHE:HB3	1:A:18:VAL:HG21	1.64	0.79
3:Q:2:SER:HB2	3:Q:3:ILE:HG12	1.64	0.79
1:C:231:ARG:CD	1:C:249:LEU:HD22	2.00	0.79
1:A:10:LEU:CD2	1:A:21:LEU:HG	2.13	0.79
1:C:122:GLU:CD	1:C:134:ARG:NH1	2.25	0.79
1:C:73:ARG:NH1	1:C:76:LEU:HD13	1.97	0.79
1:C:256:LEU:O	1:C:257:LEU:HD12	1.83	0.79
3:F:132:LEU:HD21	3:F:137:VAL:HG21	0.79	0.79
2:M:100:LEU:HD23	3:Q:3:ILE:HG21	1.62	0.79
1:A:103:VAL:O	1:A:107:PRO:HD2	1.83	0.79
1:A:259:PRO:HD2	1:A:265:LYS:HE2	1.64	0.79
1:A:24:LEU:HD23	1:A:24:LEU:O	1.83	0.78
1:D:63:LEU:HD11	1:D:68:ALA:HB2	1.65	0.78
1:D:256:LEU:O	1:D:256:LEU:HD12	1.83	0.78
2:M:153:TYR:OH	2:M:179:GLY:O	2.00	0.78
2:M:179:GLY:O	2:M:183:ALA:HB2	1.82	0.78
3:Q:69:ALA:O	3:Q:72:PRO:HD2	1.83	0.78
3:Q:160:ALA:O	3:Q:164:THR:OG1	1.99	0.78
3:F:11:ALA:HB1	3:F:16:ARG:CZ	2.12	0.78
1:A:52:ASN:OD1	1:A:54:THR:OG1	2.01	0.78
1:A:64:LEU:HD12	1:A:67:THR:H	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ASP:OD1	1:A:233:THR:OG1	1.95	0.78
1:B:11:THR:HB	1:B:59:SER:O	1.83	0.78
2:E:42:ARG:CZ	3:F:211:GLY:O	2.32	0.78
3:F:50:ILE:HG23	3:F:51:LEU:HD23	1.63	0.78
3:F:167:ARG:HG2	3:F:172:HIS:CG	2.18	0.78
1:A:16:GLY:N	1:A:17:GLY:HA2	1.98	0.78
1:B:247:LEU:HD11	1:B:249:LEU:HD23	0.80	0.78
1:B:50:HIS:ND1	1:B:57:PRO:CD	2.42	0.78
3:Q:162:MET:HE2	3:Q:192:ARG:HH12	1.47	0.78
2:M:43:MET:HE3	3:Q:210:GLN:HE21	1.47	0.78
1:B:221:GLU:O	1:B:221:GLU:HG2	1.84	0.78
1:B:234:LEU:HD23	1:B:239:LEU:CB	2.14	0.78
1:A:269:ALA:CB	1:A:270:LEU:HB2	2.14	0.78
1:D:129:SER:O	1:D:129:SER:OG	1.96	0.78
1:A:14:PHE:HE2	3:Q:8:ARG:HD2	1.46	0.78
1:A:99:VAL:HG23	1:A:135:ASP:CA	2.14	0.78
1:A:259:PRO:HG2	1:A:265:LYS:NZ	1.98	0.78
1:C:263:LEU:CD1	1:C:264:PRO:HD2	2.14	0.78
1:A:62:VAL:HG12	1:A:63:LEU:H	1.49	0.78
3:Q:21:ALA:HB3	3:Q:222:ALA:HB3	1.66	0.78
3:Q:22:GLU:CG	3:Q:222:ALA:HB1	2.15	0.78
1:D:13:ALA:CB	1:D:19:LYS:HA	2.13	0.78
3:F:166:GLN:C	3:F:168:ALA:O	2.26	0.78
1:A:62:VAL:O	1:A:63:LEU:CB	2.32	0.77
3:Q:62:LEU:HA	3:Q:63:ARG:HB2	1.65	0.77
3:Q:163:THR:CB	3:Q:167:ARG:HH12	1.97	0.77
1:A:122:GLU:HG3	1:A:123:GLU:H	1.46	0.77
1:A:147:ARG:HH12	1:A:168:THR:N	1.82	0.77
1:A:179:LEU:HD12	1:A:179:LEU:O	1.84	0.77
3:F:209:TRP:HD1	3:F:210:GLN:C	1.91	0.77
3:Q:62:LEU:HB3	3:Q:64:PHE:CB	2.15	0.77
3:F:76:LEU:O	3:F:80:ALA:N	2.12	0.77
3:Q:86:GLN:HG3	3:Q:87:ILE:CG1	2.14	0.77
1:C:124:ALA:O	1:C:127:ALA:N	2.18	0.77
3:F:84:LEU:HD23	3:F:94:LEU:HD23	0.78	0.77
1:B:247:LEU:HD13	1:B:249:LEU:HD22	1.66	0.77
3:Q:65:TRP:HE3	3:Q:117:LEU:HD13	1.49	0.77
1:A:144:GLY:O	1:A:146:LYS:N	2.18	0.77
3:F:42:GLY:O	3:F:45:LEU:CD1	2.33	0.77
1:B:18:VAL:HG22	1:B:19:LYS:N	1.98	0.77
1:D:63:LEU:HD12	1:D:67:THR:C	2.10	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:65:GLY:O	2:E:66:SER:O	2.03	0.77
1:B:265:LYS:HD2	1:B:266:THR:C	2.09	0.77
1:C:56:ARG:HB3	1:C:71:HIS:CD2	2.19	0.77
1:D:240:ARG:HG2	1:D:241:PRO:HD2	1.67	0.77
1:B:87:LEU:H	1:B:93:GLN:NE2	1.84	0.76
1:C:120:ARG:NH1	1:C:158:ARG:HD2	1.99	0.76
1:B:73:ARG:C	1:B:74:LYS:HD3	2.09	0.76
3:Q:174:THR:CG2	3:Q:177:ARG:HD2	2.13	0.76
3:F:52:ALA:O	3:F:56:LEU:HD13	1.84	0.76
1:A:109:ASN:HD22	3:Q:177:ARG:HH11	1.26	0.76
1:C:124:ALA:O	1:C:126:ALA:N	2.18	0.76
3:F:22:GLU:HG3	3:F:222:ALA:CB	2.15	0.76
3:F:84:LEU:HD21	3:F:94:LEU:HD21	1.65	0.76
3:Q:54:THR:HG22	3:Q:55:PHE:CD1	2.20	0.76
1:D:96:ALA:HB3	1:D:102:ASP:CA	2.12	0.76
1:B:30:LYS:NZ	1:B:190:GLY:O	2.19	0.76
1:B:118:ARG:HH11	1:B:118:ARG:CB	1.96	0.76
2:M:53:PHE:HB2	2:M:92:VAL:HG13	1.67	0.76
2:M:172:LEU:HD13	2:M:173:GLY:N	2.01	0.76
3:Q:22:GLU:CD	3:Q:226:VAL:HG21	2.11	0.76
3:Q:90:GLU:O	3:Q:92:ILE:N	2.18	0.76
1:A:107:PRO:O	1:A:110:LEU:HB3	1.86	0.76
3:Q:167:ARG:HG3	3:Q:167:ARG:HH11	1.51	0.76
1:C:252:ARG:HG3	1:C:257:LEU:CB	2.11	0.76
1:D:233:THR:O	1:D:236:LYS:HB2	1.86	0.76
1:A:269:ALA:HB1	1:A:270:LEU:CA	2.16	0.76
2:M:43:MET:HE3	3:Q:210:GLN:NE2	2.01	0.76
2:M:100:LEU:HD23	3:Q:3:ILE:CG2	2.15	0.76
3:F:181:SER:O	3:F:185:VAL:HG23	1.86	0.76
1:C:225:GLU:O	1:C:229:SER:OG	2.03	0.76
1:D:72:SER:H	1:D:73:ARG:HA	1.47	0.76
1:B:234:LEU:HD21	1:B:239:LEU:C	2.11	0.75
1:A:52:ASN:ND2	1:A:85:LEU:HD22	2.01	0.75
1:A:147:ARG:NH2	1:A:169:ALA:HB3	2.01	0.75
3:Q:147:LEU:HD22	3:Q:213:MET:HE1	1.68	0.75
1:D:13:ALA:HB2	1:D:19:LYS:CA	2.16	0.75
1:D:63:LEU:CD1	1:D:68:ALA:HB2	2.15	0.75
1:A:56:ARG:HD2	1:A:57:PRO:CD	2.15	0.75
1:A:128:LEU:O	1:A:182:LEU:HD13	1.83	0.75
1:D:209:ARG:NH2	1:D:221:GLU:OE2	2.18	0.75
1:B:139:HIS:HD2	3:Q:153:PHE:HB3	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ARG:NH1	1:B:221:GLU:OE2	2.20	0.75
2:E:73:THR:HG23	2:E:120:PRO:HD3	1.67	0.75
1:B:73:ARG:C	1:B:74:LYS:HZ2	1.90	0.75
1:B:76:LEU:HD22	1:B:76:LEU:N	2.02	0.75
3:F:11:ALA:HB2	3:F:16:ARG:NH1	2.01	0.75
1:D:244:VAL:CG2	1:D:261:ALA:O	2.34	0.75
1:B:80:ARG:HG2	1:B:80:ARG:HH11	1.52	0.75
1:A:14:PHE:CE2	3:Q:8:ARG:HD2	2.21	0.75
2:E:164:TYR:O	2:E:166:ASP:N	2.19	0.75
1:C:17:GLY:C	1:C:18:VAL:HG22	2.12	0.75
1:D:13:ALA:HB1	1:D:18:VAL:O	1.87	0.75
1:B:50:HIS:ND1	1:B:57:PRO:HD3	2.02	0.74
3:Q:30:PHE:CE1	3:Q:234:GLN:CG	2.47	0.74
1:D:17:GLY:O	1:D:18:VAL:CG1	2.35	0.74
3:F:188:ALA:O	3:F:191:PRO:HG2	1.86	0.74
3:F:85:ILE:HG21	3:F:92:ILE:C	2.12	0.74
1:D:71:HIS:NE2	1:D:73:ARG:CG	2.51	0.74
3:F:22:GLU:HG3	3:F:222:ALA:HB2	1.68	0.74
1:B:230:ASP:O	1:B:233:THR:OG1	2.04	0.74
3:Q:30:PHE:CD1	3:Q:234:GLN:HG2	2.20	0.74
1:C:130:ILE:HB	1:C:133:LEU:HD12	1.70	0.74
2:E:114:SER:HB2	2:E:152:THR:HB	1.69	0.74
1:A:8:GLU:CB	1:A:61:ARG:HB3	2.17	0.74
1:A:259:PRO:C	1:A:265:LYS:HE2	2.12	0.74
2:M:176:LEU:N	2:M:176:LEU:HD23	2.03	0.74
1:A:243:LEU:CD2	1:B:243:LEU:HG	2.17	0.74
1:C:265:LYS:O	1:C:266:THR:HG22	1.87	0.74
1:D:243:LEU:HD23	1:D:244:VAL:CA	2.16	0.74
1:A:24:LEU:CD1	1:A:218:VAL:CG2	2.29	0.74
1:C:15:PRO:HB3	3:F:5:SER:HA	1.70	0.74
1:A:96:ALA:O	1:A:138:THR:HG23	1.87	0.74
1:A:134:ARG:CA	1:A:135:ASP:HB2	2.18	0.74
1:A:147:ARG:HH22	1:A:169:ALA:CB	2.01	0.74
1:B:4:ILE:HG22	1:B:30:LYS:H	1.52	0.74
1:B:14:PHE:CE2	1:B:15:PRO:O	2.41	0.74
1:B:24:LEU:HD21	1:B:218:VAL:HG13	1.64	0.74
1:A:213:PHE:HE1	1:A:216:GLY:C	1.95	0.74
1:A:221:GLU:OE1	1:A:222:GLY:HA3	1.88	0.74
3:Q:90:GLU:C	3:Q:92:ILE:HG12	2.12	0.74
1:C:71:HIS:O	1:C:76:LEU:HD12	1.87	0.74
1:D:91:ASP:OD1	3:F:150:ARG:NH2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:104:GLY:C	2:E:107:THR:OG1	2.31	0.74
2:E:117:ILE:N	2:E:117:ILE:HD12	2.03	0.74
2:E:169:SER:HA	3:F:86:GLN:NE2	2.02	0.74
3:Q:170:LEU:HD13	3:Q:172:HIS:H	1.53	0.74
1:D:225:GLU:CD	1:D:225:GLU:H	1.94	0.74
1:A:10:LEU:CD2	1:A:21:LEU:CG	2.50	0.73
3:F:22:GLU:CD	3:F:222:ALA:HB2	2.12	0.73
1:B:1:MET:HG2	1:B:2:THR:H	1.53	0.73
3:Q:181:SER:O	3:Q:184:GLN:N	2.19	0.73
1:D:76:LEU:O	1:D:80:ARG:CD	2.36	0.73
1:D:243:LEU:CD2	1:D:244:VAL:N	2.50	0.73
3:F:55:PHE:O	3:F:59:ARG:HA	1.88	0.73
3:F:85:ILE:HD13	3:F:92:ILE:HG12	1.68	0.73
3:F:85:ILE:HB	3:F:94:LEU:N	2.03	0.73
3:F:132:LEU:HD22	3:F:137:VAL:HG21	1.66	0.73
1:A:257:LEU:HD22	1:A:257:LEU:N	2.04	0.73
1:D:51:LEU:O	1:D:79:TRP:NE1	2.20	0.73
1:D:187:ARG:NH1	1:D:208:ASP:OD2	2.21	0.73
1:A:76:LEU:HD13	1:A:80:ARG:CG	2.18	0.73
3:Q:91:GLY:HA3	3:Q:92:ILE:CG2	2.12	0.73
1:C:90:ALA:C	1:C:92:ASP:H	1.96	0.73
1:A:242:PRO:O	1:A:245:ILE:CG2	2.36	0.73
1:A:255:GLY:CA	1:A:257:LEU:HD21	2.18	0.73
1:B:62:VAL:CG1	1:B:79:TRP:CH2	2.71	0.73
1:B:73:ARG:O	1:B:74:LYS:HG2	1.89	0.73
3:Q:162:MET:HE1	3:Q:192:ARG:NH2	2.04	0.73
3:F:22:GLU:CG	3:F:222:ALA:HB2	2.17	0.73
1:A:249:LEU:H	1:A:249:LEU:CD2	1.95	0.73
1:C:92:ASP:OD1	3:F:192:ARG:NH1	2.17	0.73
1:A:110:LEU:HD12	1:A:111:GLY:N	2.02	0.73
3:F:85:ILE:CD1	3:F:92:ILE:HG23	2.12	0.73
1:B:10:LEU:C	1:B:11:THR:OG1	2.31	0.73
1:A:139:HIS:CD2	1:A:146:LYS:CE	2.70	0.72
1:A:180:LEU:O	1:A:184:ARG:HG3	1.88	0.72
2:M:172:LEU:O	2:M:172:LEU:HD22	1.89	0.72
3:Q:61:PRO:C	3:Q:63:ARG:HB2	2.13	0.72
3:F:50:ILE:CG2	3:F:51:LEU:HD23	2.19	0.72
3:F:209:TRP:CD1	3:F:210:GLN:N	2.57	0.72
1:C:242:PRO:O	1:C:245:ILE:CG2	2.36	0.72
1:D:265:LYS:O	1:D:266:THR:OG1	2.06	0.72
1:A:128:LEU:O	1:A:182:LEU:HD11	1.85	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:GLU:N	1:A:260:GLU:OE2	2.21	0.72
2:M:82:PRO:HG3	2:M:124:PHE:CZ	2.24	0.72
3:Q:19:PRO:CB	3:Q:222:ALA:HB2	2.19	0.72
3:Q:32:ALA:O	3:Q:36:THR:OG1	2.05	0.72
1:D:237:VAL:HG23	1:D:239:LEU:HG	1.70	0.72
1:D:256:LEU:HD12	1:D:256:LEU:C	2.14	0.72
2:E:95:PHE:HB3	2:E:99:LEU:HD12	1.70	0.72
1:A:10:LEU:HD12	1:A:11:THR:CA	2.19	0.72
1:A:76:LEU:HB2	1:A:79:TRP:CB	2.19	0.72
3:F:173:ALA:O	3:F:174:THR:HG23	1.90	0.72
1:A:76:LEU:C	1:A:79:TRP:H	1.98	0.72
1:A:108:LEU:O	1:A:108:LEU:HD23	1.90	0.72
1:B:24:LEU:CG	1:B:218:VAL:HG12	1.90	0.72
1:B:64:LEU:H	1:B:64:LEU:CD2	2.02	0.72
2:M:176:LEU:HD23	2:M:176:LEU:H	1.54	0.72
3:Q:91:GLY:N	3:Q:92:ILE:HG12	2.05	0.72
1:D:243:LEU:CD2	1:D:244:VAL:HG22	2.20	0.72
2:E:108:LEU:HD23	2:E:108:LEU:C	2.15	0.72
1:A:98:THR:HA	1:A:137:PRO:HA	1.70	0.72
1:B:10:LEU:CD1	1:B:21:LEU:HG	2.19	0.72
1:B:147:ARG:NH1	1:B:166:GLU:O	2.22	0.72
1:C:249:LEU:C	1:C:249:LEU:HD12	2.15	0.72
1:D:71:HIS:NE2	1:D:73:ARG:HG3	2.05	0.72
1:A:14:PHE:H	1:A:18:VAL:HG23	1.53	0.72
1:C:4:ILE:HD11	1:C:160:GLU:OE1	1.89	0.72
1:C:263:LEU:HD13	1:C:264:PRO:N	2.03	0.72
3:F:237:ILE:HG22	3:F:238:LEU:N	2.03	0.72
1:B:12:TYR:HA	1:B:58:GLN:OE1	1.90	0.72
2:M:62:SER:OG	2:M:188:PRO:CB	2.38	0.71
1:C:266:THR:C	1:C:267:ARG:HG2	2.14	0.71
1:D:72:SER:N	1:D:73:ARG:CA	2.51	0.71
1:B:32:GLU:OE2	1:B:209:ARG:CG	2.36	0.71
1:B:70:GLY:O	1:B:75:ASP:CB	2.32	0.71
2:E:42:ARG:NH2	3:F:143:GLU:OE1	2.19	0.71
1:B:7:ALA:O	1:B:25:SER:CB	2.38	0.71
1:B:234:LEU:HD22	1:B:234:LEU:C	2.16	0.71
1:A:8:GLU:O	1:A:9:ALA:C	2.34	0.71
1:B:73:ARG:CA	1:B:76:LEU:HD11	2.19	0.71
3:F:41:PRO:HB2	3:F:44:VAL:CG2	2.19	0.71
1:A:173:LEU:C	1:A:177:GLU:OE1	2.33	0.71
1:A:214:ARG:HG2	1:A:237:VAL:HG12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:GLU:C	1:B:25:SER:HB3	2.16	0.71
3:Q:7:ASP:OD2	3:Q:149:TYR:OH	2.07	0.71
1:D:106:GLY:N	1:D:107:PRO:CD	2.51	0.71
2:M:172:LEU:HD22	2:M:172:LEU:C	2.16	0.71
1:D:73:ARG:O	1:D:76:LEU:N	2.21	0.71
2:E:116:ALA:HB1	2:E:117:ILE:CA	2.15	0.71
1:B:247:LEU:HD12	1:B:249:LEU:CB	2.20	0.71
2:M:60:ILE:HD12	3:Q:179:LEU:HD13	1.67	0.71
1:C:263:LEU:HD13	1:C:263:LEU:C	2.15	0.71
3:F:39:PRO:O	3:F:41:PRO:HA	1.89	0.71
3:Q:238:LEU:O	3:Q:239:ALA:C	2.33	0.71
3:Q:243:LEU:HD12	3:Q:243:LEU:C	2.15	0.71
3:Q:233:LEU:HD23	3:Q:233:LEU:C	2.15	0.71
1:C:15:PRO:O	3:F:8:ARG:HD3	1.91	0.71
1:C:252:ARG:HB3	1:C:257:LEU:CD2	2.00	0.71
1:D:70:GLY:CA	1:D:75:ASP:OD2	2.38	0.71
1:B:14:PHE:CD2	1:B:15:PRO:O	2.44	0.71
2:M:199:ILE:O	2:M:202:ASP:HB3	1.91	0.71
3:F:191:PRO:O	3:F:194:LEU:N	2.24	0.71
1:A:52:ASN:HB3	1:A:163:LEU:HD12	1.73	0.70
1:A:139:HIS:HD2	1:A:146:LYS:HE2	1.55	0.70
1:A:64:LEU:HD13	1:A:65:GLY:H	1.55	0.70
1:A:112:LEU:CD1	1:A:116:GLU:CB	2.62	0.70
3:Q:62:LEU:CB	3:Q:65:TRP:N	2.54	0.70
1:D:106:GLY:O	1:D:110:LEU:HG	1.91	0.70
2:E:111:ASN:N	2:E:111:ASN:HD22	1.89	0.70
3:F:242:VAL:CG1	3:F:243:LEU:HD22	2.14	0.70
1:A:132:ASP:OD2	1:A:134:ARG:NE	2.24	0.70
1:A:143:GLY:O	1:A:146:LYS:HB2	1.91	0.70
1:A:249:LEU:HG	1:A:250:LEU:N	2.05	0.70
3:Q:227:LEU:C	3:Q:227:LEU:HD12	2.16	0.70
1:D:105:PHE:CE1	1:D:109:ASN:ND2	2.58	0.70
3:F:95:ALA:C	3:F:97:ASP:H	2.00	0.70
1:C:61:ARG:NH2	1:C:63:LEU:CD1	2.36	0.70
1:C:263:LEU:HD13	1:C:264:PRO:CD	2.21	0.70
1:A:257:LEU:HD13	1:A:257:LEU:N	2.03	0.70
1:B:62:VAL:CG1	1:B:79:TRP:HZ2	2.02	0.70
3:Q:243:LEU:HD12	3:Q:243:LEU:O	1.90	0.70
1:A:13:ALA:HB1	1:A:19:LYS:N	2.05	0.70
1:A:63:LEU:HD22	1:A:67:THR:C	2.16	0.70
2:M:59:LYS:CG	2:M:69:HIS:HD2	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ALA:O	1:C:92:ASP:N	2.25	0.70
1:A:256:LEU:O	1:A:256:LEU:HD22	1.92	0.70
1:D:76:LEU:O	1:D:80:ARG:NE	2.25	0.70
1:B:212:LEU:HB2	1:B:220:ALA:HB3	1.74	0.69
3:Q:133:ARG:HH21	3:Q:134:ARG:NH1	1.90	0.69
1:C:252:ARG:HE	1:C:257:LEU:HB3	1.57	0.69
2:E:40:GLU:OE1	3:F:198:ARG:NH1	2.19	0.69
2:E:41:ALA:C	2:E:45:LEU:HD12	2.16	0.69
3:F:42:GLY:HA2	3:F:45:LEU:HD13	1.74	0.69
3:F:51:LEU:HD21	3:F:114:CYS:SG	2.31	0.69
3:F:177:ARG:CB	3:F:180:ARG:HD2	2.21	0.69
2:M:129:LEU:O	2:M:133:ALA:N	2.25	0.69
1:C:243:LEU:HB2	1:D:243:LEU:HD11	1.74	0.69
1:D:71:HIS:CE1	1:D:73:ARG:HD2	2.26	0.69
3:Q:58:ALA:O	3:Q:59:ARG:C	2.28	0.69
3:Q:62:LEU:CB	3:Q:64:PHE:CB	2.70	0.69
1:A:24:LEU:HD11	1:A:218:VAL:HG23	0.70	0.69
1:A:99:VAL:HG22	1:A:136:ARG:C	2.16	0.69
1:A:147:ARG:NH2	1:A:169:ALA:O	2.26	0.69
1:B:114:GLU:OE2	1:B:118:ARG:NE	2.24	0.69
1:B:263:LEU:HD23	1:B:263:LEU:C	2.17	0.69
1:C:251:ALA:O	1:C:254:HIS:C	2.34	0.69
1:A:62:VAL:HG21	1:A:79:TRP:HH2	1.56	0.69
1:A:223:ALA:CB	1:A:226:ALA:HB2	2.22	0.69
1:C:73:ARG:NH1	1:C:76:LEU:CD1	2.56	0.69
1:A:8:GLU:HG3	1:A:9:ALA:N	2.07	0.69
1:B:265:LYS:HB2	1:B:267:ARG:O	1.93	0.69
3:Q:162:MET:HE3	3:Q:192:ARG:HH12	1.23	0.69
1:B:234:LEU:HD23	1:B:239:LEU:HB2	1.74	0.69
2:M:60:ILE:HD11	2:M:196:LEU:HD13	1.75	0.69
2:M:82:PRO:CG	2:M:124:PHE:CZ	2.76	0.69
1:A:134:ARG:CA	1:A:135:ASP:O	2.37	0.69
1:B:87:LEU:H	1:B:93:GLN:HE22	1.40	0.69
1:C:173:LEU:HD13	1:C:176:THR:HG21	1.74	0.69
1:D:112:LEU:HD21	1:D:116:GLU:HB2	1.73	0.69
1:D:138:THR:HA	1:D:141:LEU:HD12	1.75	0.69
1:A:208:ASP:HA	1:A:224:ALA:HB1	1.70	0.69
1:B:10:LEU:O	1:B:59:SER:C	2.36	0.69
1:B:76:LEU:HD22	1:B:76:LEU:H	1.57	0.69
1:C:263:LEU:HD13	1:C:264:PRO:HD2	1.75	0.69
1:D:71:HIS:CE1	1:D:73:ARG:NH2	2.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:TYR:HB3	1:B:21:LEU:HB3	1.73	0.68
1:C:231:ARG:CD	1:C:249:LEU:HD21	1.86	0.68
1:A:56:ARG:HD2	1:A:56:ARG:C	2.18	0.68
1:B:96:ALA:CB	1:B:102:ASP:CG	2.65	0.68
1:C:263:LEU:O	1:C:265:LYS:HG2	1.93	0.68
1:D:109:ASN:H	1:D:109:ASN:ND2	1.85	0.68
3:F:22:GLU:CD	3:F:222:ALA:CB	2.66	0.68
1:A:13:ALA:CB	1:A:19:LYS:H	2.06	0.68
2:M:83:SER:O	2:M:86:ALA:N	2.25	0.68
3:F:131:GLY:O	3:F:134:ARG:CG	2.41	0.68
1:B:63:LEU:HD22	1:B:63:LEU:H	1.59	0.68
3:Q:163:THR:CB	3:Q:167:ARG:HH22	1.98	0.68
1:A:15:PRO:HD3	1:A:18:VAL:CG2	2.24	0.68
1:A:97:THR:C	1:A:138:THR:HG1	1.97	0.68
1:A:64:LEU:HD11	1:A:67:THR:CB	2.24	0.68
1:A:255:GLY:O	1:A:257:LEU:HD11	1.63	0.68
2:M:193:GLU:HA	2:M:196:LEU:HB3	1.76	0.68
3:Q:167:ARG:C	3:Q:168:ALA:O	2.26	0.68
1:A:76:LEU:C	1:A:78:GLY:N	2.51	0.68
1:B:122:GLU:CD	1:B:134:ARG:HH12	1.98	0.68
3:Q:140:GLU:OE1	3:Q:140:GLU:N	2.19	0.68
1:A:128:LEU:O	1:A:182:LEU:HD12	1.91	0.68
1:A:139:HIS:NE2	1:A:146:LYS:NZ	2.39	0.68
1:A:177:GLU:OE2	1:B:240:ARG:NH2	2.26	0.68
1:A:246:ASP:O	1:A:249:LEU:CD1	2.26	0.68
1:C:15:PRO:O	3:F:8:ARG:CD	2.41	0.68
3:Q:66:ALA:HA	3:Q:69:ALA:CB	2.21	0.68
3:Q:238:LEU:HD13	3:Q:239:ALA:CA	2.24	0.68
1:C:15:PRO:CB	3:F:5:SER:HA	2.24	0.68
1:D:82:ARG:NH2	1:D:160:GLU:OE2	2.27	0.68
2:E:177:LYS:HZ2	3:F:86:GLN:HG2	1.59	0.68
3:F:85:ILE:HG21	3:F:92:ILE:O	1.94	0.68
1:B:230:ASP:HB3	1:B:233:THR:OG1	1.93	0.68
2:M:177:LYS:O	2:M:178:PHE:C	2.36	0.68
3:Q:19:PRO:HA	3:Q:220:PRO:HD2	1.76	0.68
1:C:172:ASP:HB2	1:C:175:GLY:H	1.58	0.68
1:C:243:LEU:O	1:C:246:ASP:N	2.27	0.68
3:F:212:GLU:O	3:F:213:MET:CB	2.42	0.68
1:A:259:PRO:HD2	1:A:265:LYS:HE3	1.74	0.67
1:B:110:LEU:HD13	1:B:157:MET:SD	2.34	0.67
3:F:212:GLU:O	3:F:213:MET:CE	2.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:LEU:HD21	1:B:218:VAL:CG1	2.22	0.67
1:B:64:LEU:H	1:B:64:LEU:HD23	1.57	0.67
1:C:152:ALA:HA	1:C:155:VAL:HG22	1.76	0.67
1:A:76:LEU:CD1	1:A:80:ARG:HG2	2.21	0.67
1:B:11:THR:O	1:B:12:TYR:HB2	1.93	0.67
1:B:50:HIS:CE1	1:B:57:PRO:CA	2.77	0.67
2:M:177:LYS:O	2:M:180:SER:N	2.18	0.67
1:D:128:LEU:HD13	1:D:152:ALA:HB2	1.77	0.67
2:E:133:ALA:O	2:E:135:ALA:N	2.26	0.67
3:F:85:ILE:HB	3:F:94:LEU:H	1.58	0.67
1:B:26:LEU:HD12	1:B:27:ALA:H	1.56	0.67
1:B:118:ARG:HB3	1:B:118:ARG:NH1	2.05	0.67
1:A:37:LEU:HD11	1:A:200:VAL:HG12	1.75	0.67
1:A:93:GLN:HE21	1:A:150:ALA:HB1	1.59	0.67
1:B:204:ALA:O	1:B:261:ALA:HB3	1.95	0.67
1:C:88:GLN:O	1:C:89:ASP:HB2	1.94	0.67
3:F:131:GLY:O	3:F:134:ARG:HG3	1.95	0.67
3:F:177:ARG:O	3:F:180:ARG:HB2	1.94	0.67
1:A:62:VAL:HG12	1:A:63:LEU:N	2.06	0.67
1:A:147:ARG:HH11	1:A:167:PRO:C	2.02	0.67
1:C:71:HIS:O	1:C:76:LEU:CD1	2.43	0.67
2:E:35:VAL:HG12	2:E:41:ALA:HB3	1.76	0.67
2:E:169:SER:HA	3:F:86:GLN:HE21	1.58	0.67
2:E:177:LYS:NZ	3:F:86:GLN:HG2	2.10	0.67
3:F:87:ILE:O	3:F:91:GLY:HA2	1.94	0.67
1:A:10:LEU:HD12	1:A:11:THR:HA	1.77	0.67
1:A:76:LEU:C	1:A:76:LEU:CD1	2.62	0.67
1:A:114:GLU:CG	1:C:2:THR:CG2	2.59	0.67
1:A:134:ARG:HA	1:A:135:ASP:C	2.13	0.67
1:A:139:HIS:CD2	1:A:146:LYS:HZ1	2.09	0.67
1:B:10:LEU:O	1:B:60:GLY:CA	2.42	0.67
3:Q:54:THR:HG22	3:Q:55:PHE:HD1	1.59	0.67
1:A:97:THR:C	1:A:138:THR:OG1	2.38	0.67
1:C:243:LEU:CD2	1:D:243:LEU:HD11	2.25	0.67
2:E:177:LYS:NZ	3:F:86:GLN:CG	2.57	0.67
3:Q:37:VAL:HG11	3:Q:42:GLY:HA3	1.75	0.67
1:B:227:VAL:O	1:B:229:SER:N	2.28	0.66
1:B:74:LYS:H	1:B:76:LEU:HD21	1.59	0.66
2:M:82:PRO:O	2:M:85:MET:HB2	1.96	0.66
3:Q:238:LEU:HD13	3:Q:238:LEU:C	2.20	0.66
2:E:166:ASP:CB	2:E:167:PRO:HD3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:169:SER:OG	2:E:170:GLY:O	2.13	0.66
1:B:73:ARG:H	1:B:74:LYS:HZ1	1.43	0.66
3:Q:85:ILE:HB	3:Q:86:GLN:CB	2.20	0.66
3:Q:238:LEU:O	3:Q:240:ALA:N	2.29	0.66
2:M:82:PRO:CG	2:M:124:PHE:CE2	2.79	0.66
1:B:63:LEU:HD13	1:B:63:LEU:N	2.10	0.66
1:C:252:ARG:HG3	1:C:257:LEU:CA	2.26	0.66
3:F:11:ALA:HB1	3:F:16:ARG:HH22	1.58	0.66
1:A:215:THR:HG22	1:A:216:GLY:H	1.61	0.66
2:M:164:TYR:C	2:M:165:PRO:O	2.38	0.66
1:C:252:ARG:CG	1:C:257:LEU:CA	2.74	0.66
1:A:242:PRO:O	1:A:245:ILE:HG22	1.96	0.66
1:A:267:ARG:HG2	1:A:268:ASP:H	1.60	0.66
1:B:9:ALA:HB3	1:B:10:LEU:O	1.95	0.66
1:B:73:ARG:H	1:B:74:LYS:NZ	1.93	0.66
1:B:90:ALA:O	1:B:94:LEU:HG	1.95	0.66
1:D:240:ARG:CG	1:D:241:PRO:HD2	2.25	0.66
3:F:139:ALA:O	3:F:142:ILE:HD11	1.95	0.66
1:A:246:ASP:O	1:A:249:LEU:HD11	1.94	0.66
1:B:73:ARG:C	1:B:74:LYS:CD	2.69	0.66
3:Q:87:ILE:HG22	3:Q:88:GLY:N	2.10	0.66
1:C:48:LEU:HD22	1:C:163:LEU:HB3	1.78	0.66
1:C:72:SER:OG	1:C:74:LYS:CE	2.44	0.66
1:C:73:ARG:NH2	1:C:80:ARG:CZ	2.55	0.66
2:E:61:PRO:CG	3:F:178:TRP:CZ3	2.79	0.66
3:F:201:GLU:CG	3:F:210:GLN:OE1	2.44	0.66
1:C:12:TYR:OH	1:C:14:PHE:CD1	2.44	0.65
1:D:264:PRO:O	1:D:265:LYS:HB2	1.96	0.65
3:F:41:PRO:HB2	3:F:44:VAL:HG23	1.77	0.65
1:A:99:VAL:CG2	1:A:135:ASP:CA	2.73	0.65
1:A:114:GLU:HG2	1:C:2:THR:HG21	1.73	0.65
1:B:50:HIS:CE1	1:B:57:PRO:CB	2.77	0.65
1:B:80:ARG:HG2	1:B:80:ARG:NH1	2.11	0.65
3:Q:62:LEU:HB2	3:Q:65:TRP:H	1.56	0.65
1:C:14:PHE:CD2	1:C:15:PRO:HD2	2.32	0.65
1:C:47:LEU:HD22	1:C:213:PHE:HZ	1.61	0.65
1:C:120:ARG:HH12	1:C:158:ARG:CD	2.02	0.65
1:C:242:PRO:O	1:C:245:ILE:HG22	1.96	0.65
1:D:38:GLY:O	1:D:44:LYS:NZ	2.25	0.65
1:A:88:GLN:N	1:A:165:ASP:OD1	2.30	0.65
1:A:107:PRO:O	1:A:112:LEU:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLN:HA	1:A:145:GLN:NE2	2.11	0.65
1:B:18:VAL:CG2	1:B:19:LYS:N	2.58	0.65
1:B:32:GLU:CG	1:B:33:SER:N	2.44	0.65
3:F:85:ILE:CB	3:F:92:ILE:HG23	2.24	0.65
1:A:8:GLU:O	1:A:10:LEU:N	2.29	0.65
1:B:263:LEU:HD23	1:B:263:LEU:O	1.96	0.65
3:Q:51:LEU:HD21	3:Q:114:CYS:SG	2.37	0.65
3:Q:65:TRP:O	3:Q:68:VAL:HG23	1.97	0.65
3:F:47:THR:O	3:F:50:ILE:CG2	2.42	0.65
1:A:147:ARG:HH22	1:A:169:ALA:CA	2.10	0.65
1:B:10:LEU:O	1:B:60:GLY:HA3	1.96	0.65
1:B:24:LEU:CD2	1:B:217:ARG:C	2.44	0.65
3:Q:23:LYS:NZ	3:Q:122:THR:O	2.29	0.65
1:C:13:ALA:HB1	1:C:18:VAL:O	1.96	0.65
1:D:17:GLY:C	1:D:18:VAL:HG12	2.22	0.65
3:F:42:GLY:CA	3:F:45:LEU:CD1	2.75	0.65
3:F:223:SER:O	3:F:225:ARG:N	2.30	0.65
1:A:144:GLY:O	1:A:145:GLN:C	2.40	0.64
1:B:50:HIS:HE1	1:B:56:ARG:C	2.05	0.64
3:Q:19:PRO:CG	3:Q:220:PRO:HG2	2.27	0.64
3:Q:22:GLU:CD	3:Q:226:VAL:CG2	2.70	0.64
1:A:231:ARG:HB3	1:A:231:ARG:HH11	1.62	0.64
2:M:78:VAL:HG11	2:M:141:VAL:HG22	1.78	0.64
1:A:99:VAL:HG23	1:A:135:ASP:N	2.12	0.64
1:B:9:ALA:HB1	1:B:11:THR:OG1	1.96	0.64
1:B:50:HIS:CD2	1:B:57:PRO:HG3	2.33	0.64
1:B:223:ALA:O	1:B:227:VAL:HG23	1.97	0.64
2:M:177:LYS:N	2:M:177:LYS:HD3	2.13	0.64
1:A:147:ARG:NH1	1:A:168:THR:N	2.44	0.64
1:B:10:LEU:C	1:B:11:THR:HG1	1.97	0.64
1:D:106:GLY:N	1:D:107:PRO:HD2	2.11	0.64
1:A:62:VAL:HG21	1:A:79:TRP:CH2	2.32	0.64
1:A:63:LEU:HD23	1:A:68:ALA:HA	1.78	0.64
1:A:87:LEU:HD23	1:A:88:GLN:HG2	1.79	0.64
1:C:246:ASP:O	1:C:250:LEU:HD23	1.97	0.64
1:D:71:HIS:CE1	1:D:73:ARG:CD	2.80	0.64
1:D:73:ARG:H	1:D:74:LYS:NZ	1.95	0.64
3:F:85:ILE:CD1	3:F:95:ALA:HA	2.15	0.64
1:A:10:LEU:O	1:A:23:ASP:HA	1.98	0.64
1:A:105:PHE:O	1:A:109:ASN:HB2	1.98	0.64
1:B:1:MET:HG2	1:B:2:THR:N	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:2:SER:HB2	3:Q:3:ILE:CG1	2.25	0.64
3:Q:62:LEU:C	3:Q:64:PHE:H	2.03	0.64
3:Q:73:LEU:O	3:Q:77:THR:HG23	1.97	0.64
1:C:74:LYS:HG3	1:C:75:ASP:HB2	1.78	0.64
1:B:38:GLY:O	1:B:44:LYS:NZ	2.20	0.64
2:M:55:LEU:HD11	2:M:75:LEU:HD23	1.78	0.64
3:Q:106:VAL:O	3:Q:110:THR:HG23	1.97	0.64
3:Q:166:GLN:O	3:Q:171:GLY:N	2.29	0.64
3:Q:223:SER:C	3:Q:225:ARG:H	2.06	0.64
1:C:73:ARG:HG2	3:F:173:ALA:O	1.97	0.64
1:D:95:PHE:CE2	3:F:213:MET:HB2	2.27	0.64
1:A:14:PHE:HB3	1:A:18:VAL:HG22	1.76	0.64
1:A:243:LEU:HD21	1:B:243:LEU:HG	1.80	0.64
2:M:40:GLU:HA	3:Q:210:GLN:HE22	1.62	0.64
1:C:242:PRO:O	1:C:245:ILE:HG23	1.98	0.64
2:E:43:MET:CG	3:F:200:LEU:HD23	2.28	0.64
1:A:76:LEU:HD12	1:A:77:THR:N	2.13	0.64
1:A:242:PRO:O	1:A:245:ILE:HG23	1.98	0.64
1:B:62:VAL:HG13	1:B:79:TRP:CZ2	2.30	0.64
3:F:84:LEU:HD23	3:F:94:LEU:HA	1.79	0.64
1:A:108:LEU:O	1:A:110:LEU:O	2.16	0.63
1:A:122:GLU:HG3	1:A:123:GLU:HG3	1.80	0.63
1:A:246:ASP:OD1	1:A:250:LEU:HD11	1.97	0.63
2:M:61:PRO:HD2	3:Q:179:LEU:CD1	2.26	0.63
3:F:140:GLU:O	3:F:144:ILE:HG13	1.98	0.63
1:A:95:PHE:CE2	3:Q:166:GLN:CG	2.82	0.63
1:A:108:LEU:HD23	1:A:108:LEU:C	2.23	0.63
1:B:227:VAL:O	1:B:228:LEU:C	2.41	0.63
1:D:13:ALA:HB1	1:D:18:VAL:C	2.24	0.63
1:A:76:LEU:CD1	1:A:80:ARG:CG	2.76	0.63
1:A:109:ASN:HD21	3:Q:177:ARG:HH11	1.43	0.63
1:A:128:LEU:HD13	1:A:182:LEU:HD12	1.81	0.63
1:A:242:PRO:O	1:A:243:LEU:O	2.16	0.63
2:M:100:LEU:CD2	3:Q:3:ILE:CG2	2.72	0.63
1:C:13:ALA:O	1:C:14:PHE:CB	2.35	0.63
1:D:103:VAL:HG13	1:D:153:GLY:HA2	1.81	0.63
1:A:243:LEU:HD23	1:B:243:LEU:HG	1.79	0.63
1:B:11:THR:OG1	1:B:59:SER:O	2.15	0.63
1:C:210:VAL:HG23	1:C:224:ALA:HA	1.80	0.63
1:A:10:LEU:HD12	1:A:11:THR:N	2.14	0.63
1:A:152:ALA:O	1:A:155:VAL:CG2	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ARG:O	1:A:215:THR:C	2.41	0.63
3:Q:174:THR:OG1	3:Q:177:ARG:CB	2.47	0.63
3:Q:201:GLU:CG	3:Q:210:GLN:HG3	2.19	0.63
1:D:13:ALA:CB	1:D:18:VAL:O	2.45	0.63
1:D:139:HIS:HD2	3:F:153:PHE:CG	2.16	0.63
1:A:99:VAL:HG21	1:A:135:ASP:O	1.99	0.63
1:C:73:ARG:HD2	1:C:73:ARG:N	2.12	0.63
1:D:70:GLY:O	1:D:71:HIS:HB2	1.98	0.63
3:F:56:LEU:N	3:F:56:LEU:HD12	2.13	0.63
1:A:267:ARG:HG2	1:A:268:ASP:N	2.13	0.63
1:D:13:ALA:CA	1:D:19:LYS:HA	2.29	0.63
1:D:230:ASP:OD2	1:D:233:THR:OG1	2.15	0.63
3:Q:163:THR:HG22	3:Q:167:ARG:NH1	2.11	0.63
1:C:72:SER:OG	1:C:74:LYS:HE3	1.99	0.63
1:D:186:LEU:HD22	1:D:191:MET:HE3	1.79	0.63
1:B:96:ALA:HB2	1:B:102:ASP:CG	2.24	0.63
1:B:264:PRO:O	1:B:265:LYS:HB3	1.98	0.63
3:F:92:ILE:HG13	3:F:93:GLY:N	2.08	0.63
1:A:214:ARG:CG	1:A:237:VAL:HG12	2.29	0.62
3:Q:62:LEU:HB3	3:Q:64:PHE:HB2	1.80	0.62
3:F:176:ARG:O	3:F:178:TRP:N	2.31	0.62
1:A:209:ARG:HH11	1:A:209:ARG:HG3	1.63	0.62
1:A:244:VAL:CG1	1:A:245:ILE:N	2.61	0.62
1:C:242:PRO:O	1:C:243:LEU:C	2.41	0.62
2:M:58:LEU:O	2:M:70:PRO:HD2	1.98	0.62
2:M:74:GLY:HA3	2:M:145:ALA:HB2	1.81	0.62
1:D:97:THR:HG21	3:F:126:ALA:CB	2.29	0.62
1:D:71:HIS:CG	1:D:72:SER:H	2.18	0.62
3:F:87:ILE:HG22	3:F:89:PRO:HA	1.80	0.62
1:A:52:ASN:HD21	1:A:85:LEU:HD22	1.64	0.62
1:B:227:VAL:C	1:B:229:SER:H	2.08	0.62
2:M:172:LEU:O	2:M:175:ALA:HB3	1.98	0.62
1:D:52:ASN:C	1:D:52:ASN:OD1	2.42	0.62
2:E:61:PRO:CD	3:F:178:TRP:CE3	2.72	0.62
1:A:56:ARG:CD	1:A:57:PRO:N	2.51	0.62
1:B:52:ASN:OD1	1:B:53:GLY:N	2.32	0.62
3:Q:33:LEU:O	3:Q:36:THR:OG1	2.17	0.62
1:D:71:HIS:N	1:D:75:ASP:HB2	2.14	0.62
1:A:259:PRO:CD	1:A:265:LYS:HE2	2.30	0.62
3:Q:240:ALA:O	3:Q:243:LEU:HD23	2.00	0.62
3:F:209:TRP:CD1	3:F:210:GLN:C	2.73	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ALA:HB1	1:B:102:ASP:CG	2.24	0.62
1:B:244:VAL:CG2	1:B:245:ILE:N	2.33	0.62
1:C:54:THR:HG21	3:F:164:THR:HG23	1.81	0.62
1:C:249:LEU:HG	1:C:250:LEU:HD22	1.82	0.62
1:D:16:GLY:H	1:D:18:VAL:HG12	1.65	0.62
2:E:33:LYS:H	2:E:33:LYS:HD2	1.63	0.61
1:C:252:ARG:HG3	1:C:257:LEU:HA	1.82	0.61
1:D:13:ALA:HB2	1:D:19:LYS:HB3	1.81	0.61
2:E:182:PHE:CE1	3:F:78:THR:HG21	2.36	0.61
3:F:59:ARG:O	3:F:60:VAL:C	2.43	0.61
1:A:76:LEU:C	1:A:78:GLY:H	2.08	0.61
3:Q:159:ALA:O	3:Q:163:THR:OG1	2.18	0.61
1:C:265:LYS:C	1:C:266:THR:CG2	2.74	0.61
3:F:84:LEU:HD21	3:F:94:LEU:CG	2.30	0.61
1:B:11:THR:O	1:B:57:PRO:HB3	2.00	0.61
2:M:30:LYS:HA	2:M:33:LYS:HG2	1.82	0.61
1:C:120:ARG:HG2	1:C:120:ARG:NH1	2.08	0.61
1:A:134:ARG:O	1:A:134:ARG:HG2	1.99	0.61
1:B:72:SER:O	1:B:73:ARG:HD2	2.01	0.61
1:C:178:GLN:HE21	1:C:178:GLN:C	2.08	0.61
3:F:125:ALA:O	3:F:128:LEU:N	2.34	0.61
1:A:269:ALA:HB1	1:A:270:LEU:HA	1.81	0.61
1:C:214:ARG:CG	1:C:215:THR:H	2.13	0.61
1:D:71:HIS:N	1:D:75:ASP:CG	2.58	0.61
3:F:174:THR:C	3:F:176:ARG:H	2.08	0.61
1:A:135:ASP:HA	1:A:136:ARG:O	2.01	0.61
1:B:40:ASN:CG	1:B:41:GLY:H	2.09	0.61
2:M:171:PHE:O	2:M:173:GLY:N	2.34	0.61
3:Q:22:GLU:CG	3:Q:222:ALA:CB	2.79	0.61
1:A:214:ARG:O	1:A:217:ARG:N	2.22	0.61
1:B:9:ALA:CB	1:B:10:LEU:HA	2.05	0.61
1:B:26:LEU:HD12	1:B:26:LEU:C	2.26	0.61
3:Q:2:SER:C	3:Q:3:ILE:HG13	2.26	0.61
3:Q:86:GLN:CG	3:Q:87:ILE:HG13	2.27	0.61
3:Q:238:LEU:HD12	3:Q:239:ALA:N	1.95	0.61
2:E:162:LEU:HD13	2:E:171:PHE:CD1	2.36	0.61
3:F:97:ASP:HB2	3:F:98:GLY:HA2	1.82	0.61
1:B:213:PHE:HB3	1:B:218:VAL:HA	1.83	0.61
1:B:69:THR:C	1:B:75:ASP:OD2	2.43	0.60
1:C:72:SER:O	1:C:76:LEU:CB	2.48	0.60
1:D:70:GLY:N	1:D:75:ASP:OD2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:LEU:HD22	1:D:244:VAL:HG22	1.82	0.60
3:F:32:ALA:O	3:F:36:THR:OG1	2.19	0.60
3:F:155:LEU:HD23	3:F:189:LEU:HD11	1.81	0.60
1:A:99:VAL:CG2	1:A:136:ARG:N	2.61	0.60
3:F:85:ILE:CD1	3:F:92:ILE:HG12	2.31	0.60
1:A:259:PRO:CD	1:A:265:LYS:CE	2.76	0.60
1:B:107:PRO:HA	1:B:110:LEU:HB3	1.82	0.60
3:F:85:ILE:HD12	3:F:95:ALA:N	2.15	0.60
1:A:8:GLU:HG3	1:A:9:ALA:H	1.65	0.60
1:A:244:VAL:HG13	1:A:245:ILE:H	1.62	0.60
1:C:64:LEU:N	1:C:67:THR:O	2.34	0.60
1:D:165:ASP:O	1:D:166:GLU:C	2.42	0.60
2:M:183:ALA:O	2:M:187:ILE:HD12	2.00	0.60
1:D:13:ALA:HA	1:D:18:VAL:O	2.01	0.60
1:A:259:PRO:HG2	1:A:265:LYS:HZ1	1.65	0.60
3:Q:91:GLY:C	3:Q:92:ILE:HG23	2.25	0.60
1:C:14:PHE:CG	1:C:15:PRO:HD3	2.36	0.60
3:F:215:VAL:O	3:F:216:LEU:HD23	2.02	0.60
3:F:237:ILE:O	3:F:239:ALA:N	2.35	0.60
2:M:173:GLY:O	2:M:177:LYS:HG2	2.02	0.60
3:Q:14:HIS:HD1	3:Q:15:TRP:HD1	1.50	0.60
1:A:147:ARG:HH22	1:A:169:ALA:N	2.00	0.60
1:B:18:VAL:CG2	1:B:19:LYS:H	2.14	0.60
1:B:86:VAL:HA	1:B:93:GLN:HE22	1.66	0.60
3:F:73:LEU:HA	3:F:76:LEU:HG	1.83	0.60
1:A:56:ARG:CD	1:A:57:PRO:CD	2.80	0.60
2:M:61:PRO:CG	3:Q:179:LEU:HB2	2.32	0.60
2:E:39:PRO:HB2	3:F:211:GLY:HA2	1.83	0.60
1:A:107:PRO:HG3	1:A:156:ALA:O	2.02	0.60
1:B:231:ARG:O	1:B:234:LEU:HD12	2.02	0.60
1:C:26:LEU:HD12	1:C:27:ALA:H	1.67	0.60
1:A:46:THR:HA	1:A:49:LEU:HD12	1.83	0.59
1:A:128:LEU:C	1:A:182:LEU:HD13	2.27	0.59
1:A:132:ASP:OD1	1:A:134:ARG:NH1	2.35	0.59
1:C:249:LEU:CD1	1:C:250:LEU:HD22	2.32	0.59
1:D:260:GLU:H	1:D:260:GLU:CD	2.10	0.59
2:E:43:MET:HG3	3:F:200:LEU:HD23	1.84	0.59
1:A:185:GLY:O	1:A:188:ALA:CB	2.48	0.59
1:A:201:GLU:OE2	1:A:205:ALA:HB2	2.02	0.59
1:B:204:ALA:HB1	1:B:261:ALA:CB	2.32	0.59
1:B:234:LEU:HD23	1:B:239:LEU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:208:ASN:C	3:Q:208:ASN:HD22	2.10	0.59
1:D:244:VAL:HG11	1:D:262:PRO:O	2.01	0.59
2:E:41:ALA:HB1	2:E:45:LEU:HD11	1.83	0.59
3:F:15:TRP:CZ2	3:F:57:GLY:CA	2.85	0.59
1:B:11:THR:N	1:B:22:ASP:O	2.33	0.59
1:B:61:ARG:HH21	1:B:71:HIS:HE1	1.47	0.59
3:F:223:SER:C	3:F:225:ARG:H	2.10	0.59
1:A:168:THR:HG21	1:A:176:THR:HG23	1.85	0.59
1:A:265:LYS:O	1:A:265:LYS:HG2	2.01	0.59
3:Q:22:GLU:HG3	3:Q:222:ALA:CB	2.33	0.59
1:C:199:ASP:HB3	1:C:202:LEU:HB3	1.83	0.59
1:B:227:VAL:C	1:B:229:SER:N	2.56	0.59
3:Q:168:ALA:C	3:Q:170:LEU:N	2.43	0.59
1:C:124:ALA:C	1:C:126:ALA:N	2.60	0.59
2:E:116:ALA:HB2	2:E:120:PRO:HG2	1.84	0.59
3:Q:167:ARG:HG3	3:Q:167:ARG:NH1	2.17	0.59
1:C:14:PHE:CD2	1:C:15:PRO:CD	2.86	0.59
1:C:14:PHE:CG	1:C:15:PRO:CD	2.86	0.59
1:B:74:LYS:N	1:B:76:LEU:HD21	2.16	0.59
3:Q:21:ALA:HB3	3:Q:222:ALA:CB	2.32	0.59
3:Q:143:GLU:OE2	3:Q:212:GLU:O	2.20	0.59
3:F:11:ALA:HB2	3:F:16:ARG:CZ	2.33	0.59
3:F:71:LEU:HD13	3:F:74:GLY:HA3	1.85	0.59
1:A:247:LEU:CA	1:A:250:LEU:HD12	2.27	0.59
2:E:61:PRO:HG3	3:F:178:TRP:CE3	2.38	0.59
3:F:201:GLU:HG3	3:F:210:GLN:OE1	2.03	0.59
3:F:242:VAL:C	3:F:244:LEU:H	2.10	0.59
1:A:242:PRO:O	1:A:243:LEU:C	2.45	0.59
2:E:7:TYR:OH	3:F:79:GLY:HA3	2.02	0.59
2:E:39:PRO:HB2	3:F:211:GLY:CA	2.33	0.59
2:E:169:SER:CA	3:F:86:GLN:HG3	2.33	0.59
3:F:209:TRP:CD1	3:F:209:TRP:C	2.81	0.59
1:A:132:ASP:HA	1:A:134:ARG:CB	2.31	0.58
1:A:168:THR:CG2	1:A:176:THR:HG23	2.32	0.58
1:A:261:ALA:O	1:A:263:LEU:O	2.21	0.58
2:E:117:ILE:O	2:E:117:ILE:HG22	2.03	0.58
1:A:252:ARG:HA	1:A:257:LEU:HB2	1.86	0.58
2:M:71:THR:O	2:M:73:THR:N	2.36	0.58
3:Q:82:VAL:HA	3:Q:85:ILE:CD1	2.29	0.58
3:Q:227:LEU:HG	3:Q:228:GLY:N	2.18	0.58
1:C:98:THR:HG22	1:C:100:PHE:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:TRP:O	1:D:79:TRP:HD1	1.85	0.58
3:F:77:THR:HA	3:F:80:ALA:HB3	1.84	0.58
1:A:10:LEU:HD21	1:A:22:ASP:N	2.17	0.58
1:A:96:ALA:HB1	1:A:101:GLU:HG2	1.86	0.58
2:E:166:ASP:HB2	2:E:167:PRO:HD3	1.82	0.58
3:F:139:ALA:O	3:F:142:ILE:CG1	2.51	0.58
1:A:133:LEU:N	1:A:134:ARG:HB2	2.17	0.58
1:B:21:LEU:C	1:B:22:ASP:O	2.44	0.58
3:Q:15:TRP:C	3:Q:16:ARG:HD3	2.28	0.58
1:D:51:LEU:O	1:D:79:TRP:CZ2	2.57	0.58
1:B:234:LEU:HD21	1:B:239:LEU:O	2.03	0.58
3:Q:16:ARG:HD2	3:Q:122:THR:O	2.03	0.58
3:Q:54:THR:CG2	3:Q:55:PHE:CE1	2.85	0.58
1:A:108:LEU:C	1:A:110:LEU:O	2.46	0.58
1:C:73:ARG:CG	3:F:173:ALA:O	2.52	0.58
1:A:10:LEU:HD12	1:A:10:LEU:C	2.29	0.58
1:B:9:ALA:HB1	1:B:10:LEU:C	2.28	0.58
1:B:69:THR:CB	1:B:75:ASP:OD2	2.48	0.58
3:Q:19:PRO:CD	3:Q:220:PRO:HG2	2.33	0.58
1:D:13:ALA:CA	1:D:18:VAL:O	2.52	0.58
1:D:252:ARG:HB3	1:D:253:ASP:OD2	2.03	0.58
2:E:54:VAL:O	2:E:55:LEU:C	2.47	0.58
1:A:13:ALA:HB2	1:A:19:LYS:HA	1.85	0.58
1:A:174:ALA:HA	1:A:177:GLU:OE1	2.03	0.58
1:C:265:LYS:O	1:C:266:THR:CG2	2.51	0.58
1:A:52:ASN:HD22	1:A:85:LEU:HB2	1.67	0.58
1:B:75:ASP:O	1:B:78:GLY:N	2.36	0.58
1:B:106:GLY:O	1:B:110:LEU:HB2	2.04	0.58
3:Q:65:TRP:CD1	3:Q:66:ALA:N	2.72	0.58
3:Q:86:GLN:C	3:Q:87:ILE:CG1	2.77	0.58
3:F:201:GLU:HB2	3:F:210:GLN:OE1	2.03	0.58
2:E:4:MET:CE	3:F:109:ALA:HB1	2.34	0.58
1:A:14:PHE:H	1:A:18:VAL:HG22	1.69	0.57
1:B:24:LEU:CG	1:B:218:VAL:N	2.64	0.57
3:Q:180:ARG:HH11	3:Q:180:ARG:CG	2.17	0.57
1:A:128:LEU:O	1:A:129:SER:HB3	2.03	0.57
1:A:252:ARG:CB	1:A:257:LEU:HB2	2.34	0.57
1:C:224:ALA:C	1:C:228:LEU:HD12	2.24	0.57
3:F:139:ALA:O	3:F:143:GLU:HG3	2.04	0.57
3:F:142:ILE:HD12	3:F:143:GLU:HG3	1.85	0.57
3:F:223:SER:C	3:F:225:ARG:N	2.59	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:GLY:O	1:B:112:LEU:HD12	2.04	0.57
2:E:169:SER:HB2	3:F:86:GLN:CG	2.14	0.57
1:A:51:LEU:O	1:A:79:TRP:CZ2	2.57	0.57
3:Q:176:ARG:HG3	3:Q:176:ARG:HH11	1.69	0.57
1:C:75:ASP:O	1:C:79:TRP:N	2.28	0.57
1:C:263:LEU:CG	1:C:264:PRO:HD2	2.34	0.57
3:Q:33:LEU:O	3:Q:37:VAL:N	2.28	0.57
1:A:131:SER:O	1:A:132:ASP:HB2	2.04	0.57
1:A:166:GLU:HB3	1:A:169:ALA:HB2	1.86	0.57
1:B:13:ALA:C	1:B:20:ALA:HB2	2.29	0.57
2:M:177:LYS:NZ	3:Q:87:ILE:HG21	2.20	0.57
1:C:124:ALA:O	1:C:125:LEU:C	2.48	0.57
1:D:94:LEU:O	3:F:150:ARG:NE	2.38	0.57
3:F:144:ILE:O	3:F:148:THR:OG1	2.13	0.57
1:A:64:LEU:HD12	1:A:64:LEU:H	1.69	0.57
1:A:256:LEU:N	1:A:257:LEU:HD13	2.17	0.57
1:B:13:ALA:HA	1:B:20:ALA:N	2.19	0.57
1:B:95:PHE:CG	1:B:96:ALA:N	2.73	0.57
1:B:101:GLU:O	3:Q:215:VAL:HG13	2.04	0.57
3:Q:40:PHE:CD2	3:Q:40:PHE:N	2.73	0.57
3:Q:60:VAL:HG13	3:Q:60:VAL:O	2.04	0.57
1:D:71:HIS:H	1:D:75:ASP:CG	2.12	0.57
1:D:85:LEU:HD12	1:D:86:VAL:H	1.70	0.57
1:D:166:GLU:OE1	1:D:198:HIS:ND1	2.36	0.57
3:F:131:GLY:O	3:F:134:ARG:HG2	2.05	0.57
1:A:39:PRO:HG2	1:A:42:ALA:HB2	1.86	0.57
1:A:99:VAL:CG2	1:A:136:ARG:C	2.65	0.57
3:Q:54:THR:HG22	3:Q:55:PHE:CE1	2.39	0.57
1:D:260:GLU:O	1:D:260:GLU:HG2	2.05	0.57
1:A:13:ALA:CB	1:A:19:LYS:HA	2.35	0.57
1:A:255:GLY:CA	1:A:257:LEU:CD2	2.83	0.57
1:B:245:ILE:HD12	1:B:245:ILE:O	2.05	0.57
3:Q:86:GLN:O	3:Q:87:ILE:HG13	2.03	0.57
2:E:52:ALA:O	2:E:55:LEU:HB3	2.04	0.57
3:F:195:THR:OG1	3:F:196:ARG:N	2.38	0.57
1:A:141:LEU:CD1	1:A:145:GLN:HB2	2.35	0.57
3:Q:86:GLN:O	3:Q:87:ILE:HD12	2.04	0.57
3:Q:170:LEU:HD13	3:Q:170:LEU:C	2.30	0.57
1:C:176:THR:O	1:C:180:LEU:HG	2.05	0.57
2:E:177:LYS:O	2:E:181:VAL:HG23	2.05	0.57
2:M:177:LYS:HD3	2:M:177:LYS:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:GLY:C	1:C:19:LYS:H	2.11	0.56
1:A:134:ARG:H	1:A:135:ASP:HB2	1.63	0.56
1:A:199:ASP:O	1:A:202:LEU:HB3	2.04	0.56
3:Q:61:PRO:HG2	3:Q:62:LEU:H	1.70	0.56
2:E:71:THR:O	2:E:193:GLU:OE2	2.23	0.56
2:E:114:SER:HB3	2:E:156:THR:HG23	1.87	0.56
2:E:177:LYS:HZ2	3:F:86:GLN:CG	2.18	0.56
1:A:98:THR:OG1	1:A:99:VAL:N	2.38	0.56
1:B:140:MET:SD	3:Q:8:ARG:HB2	2.45	0.56
2:M:178:PHE:CE1	3:Q:82:VAL:HG21	2.41	0.56
1:C:231:ARG:NH1	1:C:250:LEU:CD2	2.66	0.56
1:C:256:LEU:HD23	1:C:258:ALA:H	1.70	0.56
1:C:256:LEU:HD23	1:C:258:ALA:CA	2.34	0.56
1:D:14:PHE:CD2	1:D:15:PRO:N	2.73	0.56
1:D:71:HIS:CG	1:D:72:SER:N	2.72	0.56
1:D:128:LEU:HA	1:D:182:LEU:HD22	1.86	0.56
2:E:29:LEU:HD12	2:E:33:LYS:NZ	2.20	0.56
3:F:6:ILE:HG12	3:F:64:PHE:HZ	1.70	0.56
1:A:125:LEU:CD2	1:A:130:ILE:CD1	2.41	0.56
1:A:246:ASP:O	1:A:250:LEU:HD12	2.05	0.56
1:D:18:VAL:O	1:D:18:VAL:HG13	2.03	0.56
2:E:30:LYS:HA	2:E:33:LYS:CD	2.36	0.56
1:A:184:ARG:O	1:A:187:ARG:HB3	2.06	0.56
3:F:132:LEU:CD2	3:F:137:VAL:CB	2.83	0.56
1:A:15:PRO:HD2	1:A:18:VAL:H	1.69	0.56
1:C:11:THR:HA	1:C:21:LEU:O	2.04	0.56
1:B:6:ALA:HB3	1:B:63:LEU:HD21	1.88	0.56
1:B:114:GLU:CD	1:B:118:ARG:HD2	2.30	0.56
3:F:42:GLY:C	3:F:45:LEU:HD12	2.30	0.56
1:A:133:LEU:N	1:A:134:ARG:HA	2.21	0.56
2:M:172:LEU:HD13	2:M:172:LEU:C	2.30	0.56
1:B:164:LEU:HD23	1:B:167:PRO:HB3	1.88	0.56
1:B:244:VAL:HG22	1:B:245:ILE:HG13	1.88	0.56
3:Q:44:VAL:O	3:Q:48:VAL:HG23	2.06	0.56
3:Q:207:ARG:C	3:Q:209:TRP:H	2.14	0.56
1:C:5:LEU:HD21	1:C:51:LEU:HD22	1.88	0.56
1:D:13:ALA:HB2	1:D:19:LYS:CB	2.35	0.56
1:A:10:LEU:HD23	1:A:24:LEU:CB	2.30	0.56
1:A:56:ARG:HD3	1:A:57:PRO:HD2	1.87	0.56
1:A:64:LEU:HD12	1:A:67:THR:N	2.19	0.56
1:C:47:LEU:HD22	1:C:213:PHE:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:42:ARG:NH2	3:F:212:GLU:HA	2.21	0.56
2:E:53:PHE:HE2	3:F:3:ILE:HD12	1.69	0.56
3:F:55:PHE:O	3:F:59:ARG:N	2.35	0.56
1:A:76:LEU:O	1:A:76:LEU:HD12	2.06	0.55
1:B:82:ARG:CZ	1:B:160:GLU:OE2	2.48	0.55
2:M:176:LEU:O	2:M:180:SER:OG	2.23	0.55
3:Q:55:PHE:CD1	3:Q:55:PHE:N	2.72	0.55
1:C:42:ALA:O	1:C:213:PHE:HD2	1.88	0.55
1:D:12:TYR:O	1:D:20:ALA:N	2.38	0.55
3:F:172:HIS:NE2	3:F:178:TRP:CD1	2.74	0.55
1:A:246:ASP:HA	1:A:249:LEU:CD1	2.36	0.55
1:A:249:LEU:HD23	1:A:249:LEU:N	2.05	0.55
3:Q:162:MET:CE	3:Q:192:ARG:NH2	2.65	0.55
2:E:30:LYS:HG3	2:E:30:LYS:O	2.06	0.55
3:F:167:ARG:HG2	3:F:172:HIS:ND1	2.21	0.55
1:A:32:GLU:OE1	1:A:32:GLU:HA	2.05	0.55
1:B:225:GLU:O	1:B:226:ALA:HB3	2.05	0.55
2:M:174:ALA:HA	2:M:177:LYS:HG2	1.87	0.55
1:C:128:LEU:HA	1:C:182:LEU:HD13	1.88	0.55
2:E:10:VAL:HG22	3:F:35:VAL:HG12	1.88	0.55
1:A:15:PRO:HD2	1:A:18:VAL:N	2.21	0.55
1:A:56:ARG:CD	1:A:57:PRO:HD2	2.37	0.55
1:A:96:ALA:CB	1:A:101:GLU:HG2	2.36	0.55
1:A:96:ALA:HB3	1:A:101:GLU:HG3	1.89	0.55
1:A:110:LEU:CD1	1:A:111:GLY:H	2.15	0.55
2:M:180:SER:HA	2:M:183:ALA:CB	2.37	0.55
3:Q:86:GLN:O	3:Q:87:ILE:CG1	2.54	0.55
1:D:230:ASP:CG	1:D:233:THR:HB	2.31	0.55
3:F:47:THR:C	3:F:50:ILE:HG22	2.29	0.55
3:F:85:ILE:CG2	3:F:92:ILE:HG23	2.35	0.55
1:A:24:LEU:CD1	1:A:218:VAL:H	2.06	0.55
1:A:64:LEU:HD13	1:A:65:GLY:N	2.22	0.55
1:A:179:LEU:HD11	1:A:183:LEU:CD2	2.36	0.55
1:A:248:ALA:HA	1:A:251:ALA:HB3	1.88	0.55
1:B:138:THR:C	1:B:140:MET:H	2.14	0.55
3:Q:163:THR:HB	3:Q:167:ARG:CZ	2.35	0.55
3:F:50:ILE:HG23	3:F:51:LEU:HD22	1.86	0.55
1:A:10:LEU:HD23	1:A:24:LEU:H	1.72	0.55
1:A:141:LEU:HD12	1:A:145:GLN:HB2	1.89	0.55
1:A:270:LEU:O	1:A:270:LEU:HD23	2.06	0.55
1:B:128:LEU:HD22	1:B:148:ARG:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:87:ILE:CG2	3:Q:88:GLY:N	2.68	0.55
3:Q:140:GLU:H	3:Q:140:GLU:CD	2.12	0.55
1:D:134:ARG:HH21	3:F:218:THR:HG21	1.70	0.55
1:D:137:PRO:HD3	3:F:16:ARG:NH2	2.22	0.55
1:B:10:LEU:O	1:B:11:THR:CB	2.55	0.55
1:B:232:ALA:O	1:B:235:ALA:HB3	2.07	0.55
3:Q:70:VAL:O	3:Q:73:LEU:N	2.39	0.55
3:Q:135:TRP:N	3:Q:135:TRP:CD1	2.74	0.55
3:Q:238:LEU:CD1	3:Q:239:ALA:CA	2.81	0.55
1:D:70:GLY:H	1:D:75:ASP:CG	2.14	0.55
3:F:116:LEU:HD12	3:F:117:LEU:HD12	1.88	0.55
1:A:144:GLY:C	1:A:146:LYS:N	2.62	0.55
1:C:17:GLY:O	1:C:19:LYS:N	2.36	0.55
1:D:237:VAL:O	1:D:238:ALA:HB3	2.06	0.55
2:E:30:LYS:HB2	2:E:33:LYS:HZ3	1.72	0.55
2:E:42:ARG:CZ	3:F:212:GLU:HA	2.37	0.55
2:E:104:GLY:CA	2:E:107:THR:HG1	2.16	0.55
1:B:120:ARG:NH2	1:B:158:ARG:NE	2.49	0.55
1:C:64:LEU:HD12	1:C:69:THR:HG22	1.89	0.55
1:D:51:LEU:O	1:D:79:TRP:CE2	2.60	0.55
1:A:76:LEU:O	1:A:79:TRP:CA	2.54	0.55
1:A:86:VAL:HB	1:A:164:LEU:HB3	1.88	0.55
1:B:10:LEU:CD2	1:B:21:LEU:HD21	2.37	0.55
1:B:265:LYS:HD3	1:B:267:ARG:C	2.32	0.55
2:M:171:PHE:C	2:M:171:PHE:CD2	2.85	0.55
1:C:90:ALA:C	1:C:92:ASP:N	2.64	0.55
1:D:197:THR:OG1	1:D:198:HIS:N	2.40	0.55
3:F:40:PHE:N	3:F:41:PRO:HA	2.15	0.55
3:F:42:GLY:HA2	3:F:45:LEU:HD11	1.85	0.55
3:F:70:VAL:O	3:F:73:LEU:HB3	2.06	0.55
2:M:146:PHE:CD2	2:M:147:LEU:HD23	2.42	0.54
2:M:177:LYS:NZ	3:Q:87:ILE:CG2	2.68	0.54
1:C:37:LEU:O	1:C:212:LEU:HA	2.07	0.54
1:C:198:HIS:NE2	1:D:170:GLY:O	2.40	0.54
1:A:14:PHE:C	1:A:14:PHE:CD1	2.85	0.54
1:A:78:GLY:O	1:A:82:ARG:HG2	2.07	0.54
1:A:113:SER:O	1:A:114:GLU:C	2.50	0.54
3:Q:2:SER:HA	3:Q:3:ILE:CB	2.29	0.54
2:E:137:MET:O	2:E:141:VAL:HG13	2.08	0.54
3:F:95:ALA:C	3:F:97:ASP:N	2.65	0.54
1:A:10:LEU:O	1:A:23:ASP:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:O	1:A:133:LEU:HG	2.07	0.54
1:B:64:LEU:HD23	1:B:64:LEU:O	2.07	0.54
1:B:234:LEU:CD2	1:B:239:LEU:CB	2.85	0.54
3:Q:214:ARG:HH11	3:Q:214:ARG:HG3	1.72	0.54
1:C:42:ALA:O	1:C:213:PHE:CD2	2.60	0.54
1:C:113:SER:HG	1:C:115:ALA:HB3	1.69	0.54
1:D:5:LEU:HD21	1:D:51:LEU:HB3	1.88	0.54
2:E:42:ARG:CZ	3:F:211:GLY:C	2.80	0.54
3:F:95:ALA:O	3:F:97:ASP:N	2.39	0.54
1:B:13:ALA:H	1:B:58:GLN:HE22	1.54	0.54
1:B:73:ARG:CB	1:B:74:LYS:HD3	2.37	0.54
1:C:73:ARG:HH21	1:C:80:ARG:HH11	1.35	0.54
2:E:3:ILE:HB	2:E:111:ASN:HD21	1.72	0.54
2:E:55:LEU:HD21	2:E:72:GLY:HA3	1.89	0.54
3:F:150:ARG:HG2	3:F:154:ILE:HD11	1.89	0.54
1:A:259:PRO:CG	1:A:265:LYS:HZ1	2.20	0.54
1:B:6:ALA:HB3	1:B:63:LEU:CD2	2.38	0.54
1:C:64:LEU:HD21	1:C:82:ARG:NH1	2.22	0.54
1:A:103:VAL:HG12	1:A:121:VAL:CG2	2.31	0.54
1:D:137:PRO:HD3	3:F:16:ARG:HH22	1.72	0.54
2:E:200:VAL:HG23	3:F:183:ALA:HB1	1.89	0.54
2:E:42:ARG:NE	3:F:143:GLU:OE1	2.41	0.54
2:E:53:PHE:C	2:E:53:PHE:CD2	2.85	0.54
2:E:137:MET:O	2:E:137:MET:HG3	2.07	0.54
1:A:57:PRO:HG2	1:A:60:GLY:HA3	1.90	0.54
1:A:96:ALA:CB	1:A:101:GLU:CG	2.85	0.54
1:C:173:LEU:C	1:C:176:THR:HG22	2.32	0.54
1:D:78:GLY:O	1:D:81:ARG:N	2.40	0.54
1:B:12:TYR:O	1:B:21:LEU:N	2.33	0.54
1:C:105:PHE:HD2	3:F:169:ARG:HD3	1.73	0.54
1:D:14:PHE:CD2	1:D:14:PHE:C	2.85	0.54
1:D:96:ALA:HB3	1:D:102:ASP:CG	2.32	0.54
3:F:132:LEU:HD23	3:F:132:LEU:O	2.07	0.54
3:F:172:HIS:CD2	3:F:178:TRP:HD1	2.25	0.54
1:A:24:LEU:HD12	1:A:217:ARG:C	2.30	0.54
2:E:63:VAL:O	2:E:63:VAL:HG12	2.08	0.54
1:A:105:PHE:C	1:A:105:PHE:CD2	2.85	0.53
1:C:243:LEU:CD2	1:D:243:LEU:HG	2.37	0.53
1:C:256:LEU:C	1:C:257:LEU:HD12	2.32	0.53
1:D:105:PHE:HD1	1:D:109:ASN:ND2	1.92	0.53
2:E:29:LEU:HD12	2:E:33:LYS:HZ2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:30:LYS:HA	2:E:33:LYS:HD3	1.90	0.53
2:E:61:PRO:CD	3:F:178:TRP:HZ3	2.10	0.53
3:Q:14:HIS:HD1	3:Q:15:TRP:CD1	2.25	0.53
3:Q:185:VAL:O	3:Q:189:LEU:HB2	2.08	0.53
1:B:92:ASP:OD2	3:Q:199:ARG:HD2	2.08	0.53
3:Q:82:VAL:O	3:Q:85:ILE:HG13	2.09	0.53
3:Q:223:SER:C	3:Q:225:ARG:N	2.66	0.53
3:Q:233:LEU:HD23	3:Q:233:LEU:O	2.07	0.53
1:D:98:THR:HA	1:D:137:PRO:HA	1.90	0.53
2:E:97:ALA:O	2:E:101:ALA:HA	2.08	0.53
3:F:56:LEU:O	3:F:57:GLY:C	2.52	0.53
1:A:113:SER:C	1:A:115:ALA:N	2.66	0.53
1:A:123:GLU:O	1:A:127:ALA:N	2.23	0.53
1:B:9:ALA:CB	1:B:11:THR:OG1	2.56	0.53
2:E:4:MET:O	2:E:107:THR:CG2	2.56	0.53
3:F:219:ARG:HD2	3:F:219:ARG:O	2.08	0.53
1:A:51:LEU:O	1:A:79:TRP:HZ2	1.90	0.53
1:A:99:VAL:HG23	1:A:135:ASP:HA	1.91	0.53
1:A:141:LEU:HD12	1:A:145:GLN:CB	2.38	0.53
1:B:36:ILE:HA	1:B:211:ALA:HB3	1.90	0.53
3:Q:217:SER:OG	3:Q:219:ARG:HG3	2.08	0.53
1:C:112:LEU:CB	1:C:116:GLU:HB3	2.22	0.53
1:D:200:VAL:CG1	1:D:239:LEU:HD13	2.39	0.53
3:F:236:ALA:O	3:F:239:ALA:HB3	2.08	0.53
1:A:79:TRP:CD1	1:A:79:TRP:C	2.87	0.53
1:B:73:ARG:HB2	1:B:74:LYS:HD3	1.89	0.53
1:B:132:ASP:OD1	1:B:132:ASP:N	2.42	0.53
1:B:214:ARG:HG3	1:B:215:THR:H	1.74	0.53
1:D:79:TRP:CD1	1:D:79:TRP:C	2.86	0.53
1:D:109:ASN:N	1:D:109:ASN:ND2	2.43	0.53
3:F:78:THR:C	3:F:82:VAL:HG13	2.33	0.53
1:A:133:LEU:N	1:A:134:ARG:CA	2.72	0.53
1:B:4:ILE:HD12	1:B:4:ILE:O	2.08	0.53
1:C:36:ILE:HG13	1:C:36:ILE:O	2.09	0.53
1:C:58:GLN:H	1:C:58:GLN:CD	2.10	0.53
1:A:50:HIS:CD2	1:A:57:PRO:HD3	2.43	0.53
1:A:252:ARG:HG2	1:A:257:LEU:HB2	1.89	0.53
1:B:103:VAL:HG13	1:B:153:GLY:HA2	1.91	0.53
1:C:51:LEU:O	1:C:83:VAL:HG11	2.09	0.53
1:C:56:ARG:HB3	1:C:71:HIS:NE2	2.24	0.53
1:C:197:THR:OG1	1:C:198:HIS:N	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:93:LEU:HA	2:E:96:GLN:HG3	1.91	0.53
1:A:246:ASP:O	1:A:250:LEU:CD1	2.57	0.53
1:B:231:ARG:O	1:B:234:LEU:CD1	2.57	0.53
2:M:83:SER:O	2:M:84:VAL:C	2.48	0.53
3:Q:167:ARG:O	3:Q:168:ALA:O	2.27	0.53
1:C:263:LEU:CD1	1:C:264:PRO:CD	2.82	0.53
3:F:238:LEU:O	3:F:242:VAL:HG12	2.09	0.53
2:M:8:LEU:HG	2:M:9:PRO:HD2	1.90	0.53
3:Q:24:SER:O	3:Q:28:LEU:HB2	2.09	0.53
3:Q:227:LEU:CG	3:Q:228:GLY:N	2.72	0.53
1:D:243:LEU:HD23	1:D:244:VAL:HG22	1.91	0.53
3:F:85:ILE:HG21	3:F:93:GLY:HA2	1.91	0.53
1:A:24:LEU:HD23	1:A:24:LEU:C	2.33	0.52
1:B:64:LEU:HD23	1:B:64:LEU:N	2.22	0.52
3:Q:206:ALA:C	3:Q:207:ARG:O	2.46	0.52
2:E:203:ALA:O	2:E:206:GLY:N	2.41	0.52
3:F:85:ILE:HG13	3:F:86:GLN:H	1.74	0.52
1:B:44:LYS:HG2	1:B:213:PHE:CZ	2.44	0.52
2:M:173:GLY:O	2:M:177:LYS:HE2	2.09	0.52
3:Q:54:THR:CG2	3:Q:55:PHE:CD1	2.91	0.52
1:C:263:LEU:CG	1:C:264:PRO:CD	2.87	0.52
2:E:204:LEU:HD11	3:F:187:ALA:HA	1.91	0.52
3:F:85:ILE:HG21	3:F:93:GLY:CA	2.38	0.52
1:B:221:GLU:O	1:B:221:GLU:OE2	2.27	0.52
3:Q:151:PHE:HA	3:Q:154:ILE:HG13	1.92	0.52
2:E:189:LEU:O	2:E:190:ALA:C	2.49	0.52
1:A:96:ALA:HB3	1:A:101:GLU:CG	2.40	0.52
2:M:82:PRO:HG3	2:M:124:PHE:CD1	2.44	0.52
3:Q:15:TRP:CE2	3:Q:57:GLY:O	2.63	0.52
1:D:157:MET:SD	3:F:207:ARG:HB3	2.50	0.52
3:F:139:ALA:O	3:F:142:ILE:HG13	2.10	0.52
1:B:204:ALA:HB1	1:B:261:ALA:HB2	1.90	0.52
1:C:49:LEU:HB3	1:C:54:THR:HB	1.92	0.52
1:D:99:VAL:O	1:D:102:ASP:N	2.38	0.52
1:D:133:LEU:HD11	1:D:145:GLN:NE2	2.24	0.52
1:D:137:PRO:CD	3:F:16:ARG:HH22	2.23	0.52
2:E:58:LEU:O	2:E:69:HIS:CE1	2.55	0.52
1:A:214:ARG:HB2	1:A:219:LEU:HD23	1.92	0.52
1:B:246:ASP:O	1:B:247:LEU:HD22	2.09	0.52
1:C:243:LEU:CB	1:D:243:LEU:HD11	2.40	0.52
1:D:37:LEU:HD12	1:D:38:GLY:N	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:43:MET:HE1	3:F:210:GLN:HG2	1.92	0.52
3:F:84:LEU:CD2	3:F:94:LEU:CG	2.86	0.52
1:A:10:LEU:CD2	1:A:24:LEU:HB3	2.33	0.52
1:B:243:LEU:N	1:B:243:LEU:CD2	2.72	0.52
2:M:174:ALA:HB1	2:M:178:PHE:CE2	2.44	0.52
2:E:104:GLY:O	2:E:108:LEU:N	2.43	0.52
2:E:169:SER:OG	2:E:170:GLY:N	2.41	0.52
3:F:56:LEU:N	3:F:56:LEU:CD1	2.73	0.52
3:Q:62:LEU:HA	3:Q:63:ARG:HB3	1.85	0.52
2:E:4:MET:C	2:E:107:THR:HG21	2.35	0.52
2:E:164:TYR:HB3	3:F:83:LEU:CD1	2.40	0.52
1:A:8:GLU:HB2	1:A:61:ARG:HD2	1.91	0.52
1:A:86:VAL:HA	1:A:93:GLN:HE22	1.75	0.52
1:B:85:LEU:HD21	1:B:87:LEU:HD21	1.91	0.52
2:M:87:VAL:O	2:M:91:ILE:HG13	2.10	0.52
3:Q:62:LEU:CB	3:Q:64:PHE:C	2.70	0.52
1:D:16:GLY:N	1:D:17:GLY:CA	2.72	0.52
1:D:117:ALA:O	1:D:121:VAL:HG23	2.10	0.52
3:F:195:THR:O	3:F:198:ARG:N	2.35	0.52
1:A:198:HIS:HB3	1:B:172:ASP:HA	1.90	0.52
2:M:59:LYS:HG3	2:M:69:HIS:CD2	2.34	0.52
3:Q:65:TRP:CD1	3:Q:66:ALA:H	2.28	0.52
3:Q:86:GLN:O	3:Q:87:ILE:CD1	2.58	0.52
3:Q:176:ARG:HH11	3:Q:176:ARG:CG	2.23	0.52
1:C:214:ARG:CG	1:C:215:THR:N	2.73	0.52
1:D:71:HIS:HE1	1:D:73:ARG:HD2	1.74	0.52
3:F:174:THR:C	3:F:176:ARG:N	2.65	0.52
3:F:212:GLU:N	3:F:212:GLU:OE1	2.40	0.52
2:M:171:PHE:C	2:M:173:GLY:H	2.18	0.51
3:Q:15:TRP:N	3:Q:16:ARG:HH21	1.99	0.51
1:C:178:GLN:CA	1:C:178:GLN:NE2	2.73	0.51
1:D:243:LEU:HD23	1:D:244:VAL:H	1.65	0.51
1:A:64:LEU:CD1	1:A:65:GLY:H	2.20	0.51
1:A:179:LEU:HD11	1:A:183:LEU:HD21	1.92	0.51
1:B:32:GLU:HG2	1:B:208:ASP:HB2	1.86	0.51
1:B:74:LYS:N	1:B:76:LEU:CD2	2.73	0.51
3:Q:10:ALA:O	3:Q:124:PRO:HG3	2.10	0.51
3:Q:133:ARG:NH2	3:Q:134:ARG:NH1	2.56	0.51
3:F:142:ILE:HD12	3:F:143:GLU:N	2.26	0.51
1:A:247:LEU:HD21	1:B:263:LEU:CD1	2.40	0.51
1:C:230:ASP:OD1	1:C:232:ALA:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:GLY:C	1:D:75:ASP:HB2	2.35	0.51
3:F:85:ILE:CB	3:F:94:LEU:H	2.22	0.51
1:A:166:GLU:OE1	1:A:198:HIS:NE2	2.43	0.51
2:E:30:LYS:O	2:E:34:ILE:HG13	2.10	0.51
3:F:15:TRP:CZ2	3:F:57:GLY:HA2	2.46	0.51
1:A:10:LEU:CD1	1:A:11:THR:HA	2.40	0.51
1:B:6:ALA:O	1:B:62:VAL:HG23	2.11	0.51
2:M:177:LYS:HZ3	3:Q:87:ILE:HG21	1.76	0.51
2:E:7:TYR:OH	3:F:79:GLY:CA	2.57	0.51
3:F:168:ALA:O	3:F:169:ARG:HB2	2.10	0.51
1:A:244:VAL:CG1	1:A:245:ILE:H	2.23	0.51
2:M:166:ASP:OD1	2:M:167:PRO:HD2	2.10	0.51
2:M:166:ASP:CG	2:M:169:SER:H	2.03	0.51
2:M:174:ALA:CA	2:M:177:LYS:HG2	2.40	0.51
3:Q:163:THR:HB	3:Q:167:ARG:NH1	2.26	0.51
1:C:231:ARG:HH11	1:C:249:LEU:CD2	2.22	0.51
1:C:252:ARG:HA	1:C:254:HIS:O	2.10	0.51
1:D:13:ALA:HA	1:D:19:LYS:HA	1.92	0.51
3:F:118:PHE:O	3:F:122:THR:HG23	2.10	0.51
1:A:8:GLU:HB2	1:A:61:ARG:CD	2.41	0.51
1:A:15:PRO:CD	1:A:18:VAL:CG1	2.86	0.51
1:A:252:ARG:CG	1:A:257:LEU:HB2	2.41	0.51
1:B:52:ASN:ND2	1:B:85:LEU:HD22	2.25	0.51
2:M:64:THR:HG23	2:M:66:SER:H	1.76	0.51
1:C:13:ALA:HA	1:C:19:LYS:HA	1.93	0.51
1:C:212:LEU:HD21	1:C:234:LEU:HD23	1.92	0.51
1:D:128:LEU:O	1:D:129:SER:HB3	2.11	0.51
1:D:145:GLN:O	1:D:149:VAL:HG23	2.10	0.51
3:F:87:ILE:HG22	3:F:88:GLY:N	2.26	0.51
3:F:106:VAL:O	3:F:110:THR:HG23	2.11	0.51
1:A:24:LEU:CD1	1:A:218:VAL:N	2.53	0.51
1:A:64:LEU:CD1	1:A:65:GLY:N	2.74	0.51
1:B:13:ALA:HA	1:B:20:ALA:CA	2.37	0.51
3:Q:55:PHE:HD1	3:Q:55:PHE:N	2.08	0.51
1:C:113:SER:OG	1:C:115:ALA:HB1	2.08	0.51
1:D:73:ARG:O	1:D:76:LEU:HB2	2.11	0.51
1:B:76:LEU:N	1:B:76:LEU:CD2	2.73	0.51
2:M:171:PHE:C	2:M:171:PHE:HD2	2.18	0.51
3:F:201:GLU:CB	3:F:210:GLN:OE1	2.59	0.51
1:A:113:SER:C	1:A:115:ALA:H	2.17	0.51
1:B:234:LEU:HD13	1:B:234:LEU:C	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:HIS:N	1:D:75:ASP:CB	2.74	0.51
1:D:252:ARG:C	1:D:253:ASP:CG	2.78	0.51
1:A:183:LEU:HD13	1:A:193:LEU:HD13	1.92	0.50
2:M:180:SER:HA	2:M:183:ALA:HB3	1.91	0.50
3:F:14:HIS:CD2	3:F:15:TRP:CD1	2.99	0.50
1:B:4:ILE:HG22	1:B:30:LYS:N	2.25	0.50
3:Q:117:LEU:O	3:Q:121:THR:OG1	2.21	0.50
1:D:75:ASP:O	1:D:79:TRP:HB3	2.10	0.50
1:D:105:PHE:HD1	1:D:105:PHE:O	1.94	0.50
3:F:42:GLY:C	3:F:45:LEU:CD1	2.85	0.50
1:B:223:ALA:HB3	1:B:225:GLU:O	2.12	0.50
2:E:65:GLY:O	2:E:66:SER:C	2.55	0.50
2:E:167:PRO:HD2	2:E:168:ALA:N	2.26	0.50
3:F:75:PHE:O	3:F:78:THR:HB	2.12	0.50
2:M:71:THR:C	2:M:73:THR:H	2.20	0.50
3:Q:54:THR:HG21	3:Q:55:PHE:HE1	1.76	0.50
1:C:64:LEU:HB2	1:C:69:THR:HG22	1.94	0.50
2:E:61:PRO:CD	3:F:178:TRP:CH2	2.72	0.50
3:F:228:GLY:O	3:F:232:THR:HG23	2.10	0.50
1:A:15:PRO:O	1:A:17:GLY:HA2	2.12	0.50
1:B:18:VAL:HG22	1:B:19:LYS:H	1.68	0.50
3:Q:224:ALA:C	3:Q:227:LEU:HB3	2.36	0.50
1:D:7:ALA:O	1:D:25:SER:HA	2.11	0.50
1:D:71:HIS:ND1	1:D:72:SER:N	2.60	0.50
1:A:243:LEU:O	1:A:246:ASP:N	2.44	0.50
2:M:1:MET:HG3	2:M:2:HIS:ND1	2.27	0.50
2:M:30:LYS:O	2:M:34:ILE:HG13	2.12	0.50
2:M:82:PRO:HD3	2:M:124:PHE:HE2	1.63	0.50
1:C:250:LEU:CD2	1:C:250:LEU:N	2.75	0.50
1:D:157:MET:CE	3:F:207:ARG:HB3	2.42	0.50
2:E:5:GLU:HA	2:E:107:THR:CG2	2.42	0.50
3:F:73:LEU:O	3:F:76:LEU:HG	2.11	0.50
3:F:172:HIS:CE1	3:F:178:TRP:NE1	2.79	0.50
1:C:12:TYR:CD2	1:C:13:ALA:O	2.65	0.50
2:E:114:SER:OG	2:E:115:MET:N	2.43	0.50
1:B:243:LEU:C	1:B:244:VAL:CG1	2.85	0.50
3:Q:175:ARG:O	3:Q:178:TRP:N	2.44	0.50
1:C:178:GLN:HE21	1:C:178:GLN:CA	2.24	0.50
1:D:230:ASP:CG	1:D:233:THR:CB	2.85	0.50
1:A:109:ASN:HD22	3:Q:177:ARG:NH1	1.94	0.49
1:A:132:ASP:CG	1:A:134:ARG:HH11	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:LYS:CD	1:B:267:ARG:C	2.85	0.49
2:M:12:HIS:O	2:M:16:TRP:N	2.45	0.49
1:D:70:GLY:C	1:D:75:ASP:OD2	2.55	0.49
2:E:37:GLU:OE1	2:E:38:ARG:HG3	2.12	0.49
2:E:65:GLY:C	2:E:66:SER:O	2.55	0.49
3:F:23:LYS:HE2	3:F:123:THR:OG1	2.11	0.49
1:A:247:LEU:HD21	1:B:263:LEU:HD12	1.94	0.49
1:B:6:ALA:HA	1:B:27:ALA:HA	1.94	0.49
1:B:109:ASN:HD22	3:Q:209:TRP:HB2	1.78	0.49
1:B:123:GLU:OE1	1:B:158:ARG:NH1	2.44	0.49
1:C:72:SER:OG	1:C:74:LYS:HB3	2.12	0.49
1:C:114:GLU:N	1:C:115:ALA:CB	2.72	0.49
1:C:265:LYS:C	1:C:266:THR:HG23	2.37	0.49
1:D:244:VAL:O	1:D:247:LEU:N	2.45	0.49
3:F:237:ILE:HG22	3:F:238:LEU:H	1.76	0.49
1:A:270:LEU:HD23	1:A:270:LEU:C	2.37	0.49
1:B:71:HIS:CD2	1:B:71:HIS:N	2.71	0.49
3:Q:163:THR:C	3:Q:167:ARG:CZ	2.86	0.49
3:Q:170:LEU:C	3:Q:170:LEU:CD1	2.85	0.49
1:C:142:SER:OG	1:C:145:GLN:HG3	2.12	0.49
1:D:35:ALA:HB2	1:D:207:ALA:HB2	1.93	0.49
1:D:71:HIS:CD2	1:D:73:ARG:HG3	2.46	0.49
1:D:250:LEU:C	1:D:252:ARG:H	2.19	0.49
2:E:125:GLY:O	2:E:129:LEU:HB2	2.11	0.49
1:A:35:ALA:HB2	1:A:195:PHE:CZ	2.47	0.49
1:A:62:VAL:O	1:A:63:LEU:HB2	2.09	0.49
1:A:255:GLY:HA3	1:A:257:LEU:CG	2.42	0.49
1:B:37:LEU:HB3	1:B:212:LEU:HD23	1.93	0.49
3:Q:19:PRO:HG2	3:Q:222:ALA:HA	1.94	0.49
3:Q:90:GLU:O	3:Q:91:GLY:C	2.56	0.49
1:C:72:SER:C	1:C:76:LEU:HB2	2.37	0.49
1:D:34:LEU:HD22	1:D:36:ILE:HD13	1.95	0.49
1:D:73:ARG:HG2	1:D:76:LEU:HD13	1.95	0.49
3:F:39:PRO:HB2	3:F:107:MET:SD	2.52	0.49
3:F:86:GLN:OE1	3:F:88:GLY:N	2.45	0.49
1:A:248:ALA:HB1	1:A:260:GLU:HB3	1.93	0.49
1:A:263:LEU:H	1:A:263:LEU:CD1	2.00	0.49
1:B:114:GLU:CD	1:B:118:ARG:CD	2.85	0.49
1:B:247:LEU:HD13	1:B:248:ALA:H	1.77	0.49
3:Q:226:VAL:O	3:Q:230:ILE:HG13	2.12	0.49
1:D:16:GLY:CA	1:D:17:GLY:C	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ASP:O	1:D:224:ALA:N	2.45	0.49
2:E:61:PRO:CG	3:F:178:TRP:CE3	2.96	0.49
2:E:176:LEU:O	2:E:176:LEU:HD23	2.13	0.49
3:F:85:ILE:CG2	3:F:94:LEU:H	2.25	0.49
1:A:87:LEU:HD23	1:A:88:GLN:N	2.27	0.49
3:Q:2:SER:CB	3:Q:3:ILE:HG12	2.39	0.49
3:Q:60:VAL:HG13	3:Q:62:LEU:O	2.13	0.49
1:C:73:ARG:CZ	1:C:76:LEU:CD1	2.84	0.49
2:E:193:GLU:O	2:E:197:THR:HG23	2.12	0.49
1:A:230:ASP:OD2	1:A:233:THR:OG1	2.27	0.49
3:Q:164:THR:N	3:Q:167:ARG:NH2	2.60	0.49
3:Q:223:SER:O	3:Q:225:ARG:N	2.46	0.49
3:Q:227:LEU:HG	3:Q:228:GLY:H	1.78	0.49
1:C:249:LEU:CG	1:C:250:LEU:CD2	2.85	0.49
2:E:200:VAL:HG23	3:F:183:ALA:CB	2.43	0.49
1:A:125:LEU:HD22	1:A:130:ILE:HD11	0.63	0.49
1:A:164:LEU:CD1	1:A:167:PRO:HG3	2.42	0.49
3:Q:2:SER:C	3:Q:3:ILE:CG1	2.86	0.49
3:Q:82:VAL:C	3:Q:85:ILE:HG12	2.36	0.49
3:Q:133:ARG:NH2	3:Q:134:ARG:HH11	2.10	0.49
3:Q:194:LEU:O	3:Q:197:ALA:HB3	2.12	0.49
1:C:56:ARG:CB	1:C:71:HIS:NE2	2.76	0.49
1:C:231:ARG:HH11	1:C:249:LEU:HD23	1.76	0.49
1:C:256:LEU:CD2	1:C:258:ALA:CA	2.89	0.49
1:C:266:THR:OG1	1:C:267:ARG:N	2.45	0.49
2:E:43:MET:HE1	3:F:210:GLN:CG	2.43	0.49
1:A:112:LEU:HD12	1:A:116:GLU:C	2.38	0.49
1:B:61:ARG:HD2	1:B:61:ARG:N	2.27	0.49
1:B:120:ARG:HH21	1:B:158:ARG:NH2	2.11	0.49
1:B:265:LYS:CD	1:B:265:LYS:C	2.85	0.49
2:M:177:LYS:N	2:M:177:LYS:CD	2.73	0.49
1:C:44:LYS:HD3	1:C:44:LYS:H	1.76	0.49
1:C:73:ARG:NH2	1:C:76:LEU:HD13	2.27	0.49
1:B:13:ALA:N	1:B:58:GLN:HE22	2.10	0.49
1:B:64:LEU:O	1:B:64:LEU:CG	2.61	0.49
1:B:79:TRP:O	1:B:83:VAL:HG23	2.13	0.49
1:B:118:ARG:HH11	1:B:118:ARG:CG	2.25	0.49
1:D:37:LEU:HD21	1:D:200:VAL:HG12	1.95	0.49
2:E:71:THR:O	2:E:193:GLU:CD	2.56	0.49
3:F:41:PRO:HB2	3:F:44:VAL:HG21	1.91	0.49
1:A:255:GLY:O	1:A:256:LEU:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:55:LEU:O	2:M:58:LEU:HB2	2.13	0.48
1:D:72:SER:H	1:D:73:ARG:HG3	1.78	0.48
1:D:95:PHE:CE2	3:F:213:MET:CB	2.96	0.48
1:A:185:GLY:O	1:A:188:ALA:N	2.46	0.48
1:B:44:LYS:HG2	1:B:213:PHE:CE2	2.48	0.48
2:M:42:ARG:HD3	3:Q:213:MET:HE2	1.95	0.48
3:Q:54:THR:CG2	3:Q:55:PHE:HE1	2.25	0.48
1:D:209:ARG:HD2	1:D:223:ALA:HA	1.95	0.48
1:D:219:LEU:HD21	1:D:236:LYS:HD2	1.95	0.48
1:A:242:PRO:HB2	1:A:245:ILE:HG22	1.96	0.48
1:B:73:ARG:C	1:B:74:LYS:CG	2.86	0.48
1:B:138:THR:O	1:B:140:MET:N	2.46	0.48
1:C:98:THR:HB	1:C:101:GLU:HG3	1.94	0.48
1:C:101:GLU:O	1:C:104:SER:HB2	2.13	0.48
1:D:212:LEU:HD11	1:D:234:LEU:HD23	1.95	0.48
2:E:19:ALA:C	2:E:113:PHE:HE1	2.20	0.48
3:F:86:GLN:OE1	3:F:87:ILE:N	2.46	0.48
1:A:14:PHE:N	1:A:18:VAL:CG2	2.72	0.48
1:A:63:LEU:CD2	1:A:68:ALA:HA	2.41	0.48
1:B:8:GLU:HA	1:B:25:SER:CB	2.28	0.48
1:B:8:GLU:HB2	1:B:61:ARG:O	2.13	0.48
1:B:10:LEU:CG	1:B:21:LEU:HD21	2.39	0.48
1:B:28:VAL:HG22	1:B:34:LEU:HD22	1.95	0.48
1:B:71:HIS:C	1:B:73:ARG:N	2.67	0.48
1:B:213:PHE:HB2	1:B:217:ARG:O	2.13	0.48
2:M:166:ASP:CB	2:M:173:GLY:HA3	2.27	0.48
3:Q:236:ALA:O	3:Q:238:LEU:N	2.46	0.48
1:D:95:PHE:HE2	3:F:213:MET:CB	2.19	0.48
2:E:55:LEU:CD1	3:F:186:ILE:HD13	2.44	0.48
2:E:108:LEU:HD23	2:E:109:GLY:CA	2.43	0.48
1:A:10:LEU:HD23	1:A:24:LEU:N	2.28	0.48
3:Q:16:ARG:HD3	3:Q:16:ARG:N	2.29	0.48
1:D:71:HIS:NE2	1:D:73:ARG:HG2	2.26	0.48
1:D:94:LEU:O	3:F:150:ARG:CZ	2.61	0.48
1:B:96:ALA:HB1	1:B:102:ASP:HB2	1.93	0.48
1:B:234:LEU:CD2	1:B:239:LEU:HB2	2.41	0.48
2:M:38:ARG:HA	2:M:39:PRO:HD2	1.64	0.48
2:M:100:LEU:HD23	3:Q:3:ILE:HG22	1.95	0.48
2:M:171:PHE:C	2:M:173:GLY:N	2.72	0.48
3:Q:43:ALA:HA	3:Q:46:VAL:HB	1.94	0.48
3:Q:170:LEU:HD12	3:Q:173:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:GLU:CG	1:C:178:GLN:N	2.77	0.48
2:E:88:LEU:O	2:E:92:VAL:HG23	2.13	0.48
1:A:76:LEU:CD1	1:A:80:ARG:HG3	2.43	0.48
1:A:110:LEU:C	1:A:112:LEU:H	2.21	0.48
1:B:135:ASP:HB3	3:Q:218:THR:HG21	1.96	0.48
2:E:39:PRO:CB	3:F:211:GLY:HA2	2.44	0.48
1:C:72:SER:HG	1:C:74:LYS:HB3	1.78	0.48
1:C:151:ILE:O	1:C:155:VAL:HG13	2.14	0.48
1:C:242:PRO:O	1:C:243:LEU:O	2.32	0.48
1:C:256:LEU:HD23	1:C:258:ALA:CB	2.41	0.48
1:D:16:GLY:N	1:D:17:GLY:HA2	2.29	0.48
3:F:148:THR:O	3:F:152:VAL:HG23	2.14	0.48
1:A:269:ALA:CB	1:A:270:LEU:CA	2.85	0.48
1:B:71:HIS:HB2	1:B:72:SER:H	1.49	0.48
2:M:2:HIS:CE1	2:M:102:HIS:HE2	2.32	0.48
3:Q:130:SER:O	3:Q:133:ARG:HB3	2.12	0.48
3:Q:212:GLU:O	3:Q:213:MET:HG3	2.13	0.48
1:C:21:LEU:HD11	1:C:50:HIS:CD2	2.48	0.48
1:C:114:GLU:H	1:C:115:ALA:HB3	1.78	0.48
1:D:157:MET:O	1:D:159:PRO:HD3	2.13	0.48
3:F:159:ALA:HB2	3:F:189:LEU:CD2	2.44	0.48
1:A:16:GLY:N	1:A:17:GLY:CA	2.73	0.48
1:A:45:SER:O	1:A:49:LEU:HG	2.13	0.48
1:A:90:ALA:O	1:A:93:GLN:HB3	2.14	0.48
1:B:147:ARG:NH2	1:B:169:ALA:O	2.45	0.48
1:B:247:LEU:HD12	1:B:249:LEU:H	1.79	0.48
1:C:98:THR:HG22	1:C:100:PHE:N	2.29	0.48
1:C:129:SER:O	1:C:129:SER:OG	2.28	0.48
1:B:165:ASP:OD1	1:B:166:GLU:HG2	2.14	0.47
2:M:122:VAL:O	2:M:126:VAL:HG23	2.14	0.47
1:D:95:PHE:CE1	1:D:105:PHE:CD2	3.02	0.47
3:F:78:THR:O	3:F:81:ALA:N	2.44	0.47
2:M:178:PHE:HE1	3:Q:82:VAL:HG21	1.79	0.47
2:M:185:THR:O	2:M:188:PRO:HD2	2.14	0.47
1:C:231:ARG:HH12	1:C:250:LEU:CD2	2.15	0.47
1:D:141:LEU:HD22	1:D:145:GLN:HB3	1.96	0.47
2:E:5:GLU:OE1	2:E:105:LEU:CA	2.57	0.47
2:E:167:PRO:HD2	2:E:168:ALA:H	1.79	0.47
1:A:179:LEU:HD12	1:A:179:LEU:C	2.39	0.47
1:A:215:THR:HG22	1:A:216:GLY:N	2.29	0.47
1:B:122:GLU:CD	1:B:134:ARG:NH1	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:62:SER:HG	2:M:188:PRO:CB	2.26	0.47
1:C:228:LEU:O	1:C:241:PRO:HB3	2.15	0.47
2:E:85:MET:HA	2:E:85:MET:HE3	1.96	0.47
3:F:95:ALA:HB1	3:F:96:PRO:HD2	1.95	0.47
3:F:205:GLY:O	3:F:206:ALA:C	2.57	0.47
3:Q:180:ARG:CG	3:Q:180:ARG:NH1	2.74	0.47
3:Q:236:ALA:C	3:Q:238:LEU:N	2.72	0.47
1:D:63:LEU:CD1	1:D:67:THR:C	2.86	0.47
1:D:209:ARG:HH21	1:D:221:GLU:CD	2.20	0.47
2:E:46:ALA:HB3	3:F:151:PHE:CD1	2.49	0.47
1:A:10:LEU:O	1:A:23:ASP:CA	2.61	0.47
1:A:128:LEU:O	1:A:128:LEU:HD13	2.14	0.47
1:A:132:ASP:OD2	1:A:134:ARG:NH1	2.47	0.47
1:A:252:ARG:CA	1:A:257:LEU:HB2	2.44	0.47
3:Q:70:VAL:HG13	3:Q:73:LEU:HD22	1.97	0.47
3:Q:213:MET:O	3:Q:215:VAL:HG23	2.14	0.47
1:C:242:PRO:HB2	1:C:245:ILE:HG22	1.96	0.47
2:E:41:ALA:O	2:E:44:THR:N	2.47	0.47
2:E:46:ALA:HB3	3:F:151:PHE:CE1	2.49	0.47
1:A:244:VAL:O	1:A:245:ILE:C	2.53	0.47
1:B:64:LEU:O	1:B:64:LEU:HG	2.13	0.47
3:Q:163:THR:C	3:Q:167:ARG:NH2	2.73	0.47
3:Q:180:ARG:HH11	3:Q:180:ARG:HG3	1.79	0.47
1:D:82:ARG:NE	1:D:160:GLU:OE2	2.48	0.47
1:D:177:GLU:HA	1:D:180:LEU:HD12	1.97	0.47
2:E:43:MET:SD	3:F:200:LEU:HD23	2.55	0.47
1:A:132:ASP:CG	1:A:134:ARG:NH1	2.72	0.47
1:A:252:ARG:CD	1:A:252:ARG:C	2.88	0.47
1:B:79:TRP:CD1	1:B:83:VAL:HG21	2.50	0.47
1:B:243:LEU:C	1:B:244:VAL:HG12	2.40	0.47
2:M:4:MET:HG3	2:M:5:GLU:N	2.29	0.47
2:M:186:GLN:HG3	2:M:186:GLN:O	2.14	0.47
3:Q:224:ALA:O	3:Q:227:LEU:HB3	2.15	0.47
1:D:114:GLU:CD	1:D:114:GLU:H	2.22	0.47
2:E:118:VAL:HG21	2:E:155:THR:HG21	1.97	0.47
3:F:45:LEU:HD12	3:F:45:LEU:N	2.08	0.47
3:F:242:VAL:HG13	3:F:243:LEU:N	2.30	0.47
1:A:21:LEU:HD11	1:A:47:LEU:HD13	1.97	0.47
1:A:233:THR:O	1:A:236:LYS:HG2	2.15	0.47
1:A:263:LEU:HD12	1:A:263:LEU:N	2.07	0.47
1:B:118:ARG:NH1	1:B:118:ARG:CG	2.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ALA:HB1	1:B:261:ALA:HB1	1.96	0.47
3:Q:62:LEU:CG	3:Q:65:TRP:N	2.57	0.47
3:Q:70:VAL:O	3:Q:71:LEU:C	2.58	0.47
1:C:21:LEU:CD1	1:C:50:HIS:CD2	2.97	0.47
1:C:64:LEU:CD2	1:C:82:ARG:NH1	2.77	0.47
3:F:14:HIS:HD2	3:F:15:TRP:HD1	1.62	0.47
3:F:42:GLY:O	3:F:43:ALA:C	2.58	0.47
1:B:51:LEU:O	1:B:83:VAL:HG11	2.15	0.47
1:B:265:LYS:CD	1:B:266:THR:C	2.85	0.47
2:M:59:LYS:CG	2:M:69:HIS:CD2	2.93	0.47
1:C:13:ALA:CB	1:C:18:VAL:O	2.63	0.47
2:E:69:HIS:C	2:E:189:LEU:HD11	2.39	0.47
3:F:30:PHE:HB3	3:F:115:CYS:SG	2.55	0.47
3:F:155:LEU:HD21	3:F:193:ALA:HB2	1.97	0.47
1:A:14:PHE:CE2	3:Q:8:ARG:CD	2.96	0.47
1:B:114:GLU:CD	1:B:118:ARG:NE	2.73	0.47
3:Q:158:GLU:HG3	3:Q:192:ARG:HH11	1.79	0.47
3:Q:163:THR:C	3:Q:167:ARG:NH1	2.73	0.47
3:Q:208:ASN:C	3:Q:208:ASN:ND2	2.73	0.47
1:D:58:GLN:CD	1:D:58:GLN:H	2.23	0.47
1:D:98:THR:HG1	1:D:136:ARG:C	2.20	0.47
3:Q:2:SER:CA	3:Q:3:ILE:CG1	2.93	0.46
3:Q:163:THR:CB	3:Q:167:ARG:NH1	2.73	0.46
1:D:31:GLY:N	1:D:192:THR:OG1	2.47	0.46
1:D:36:ILE:O	1:D:44:LYS:HD2	2.15	0.46
2:E:129:LEU:HD12	2:E:129:LEU:HA	1.48	0.46
3:F:50:ILE:HG23	3:F:51:LEU:N	2.28	0.46
3:F:225:ARG:O	3:F:228:GLY:N	2.48	0.46
1:A:86:VAL:HG13	1:A:93:GLN:NE2	2.30	0.46
1:A:145:GLN:O	1:A:149:VAL:HG23	2.15	0.46
1:B:118:ARG:HG2	3:Q:216:LEU:HD13	1.98	0.46
3:Q:61:PRO:HG2	3:Q:62:LEU:N	2.29	0.46
1:C:105:PHE:CD2	3:F:169:ARG:HD3	2.50	0.46
1:D:134:ARG:HH21	3:F:218:THR:CG2	2.27	0.46
2:E:41:ALA:HB1	2:E:45:LEU:CD1	2.44	0.46
1:A:56:ARG:HD2	1:A:57:PRO:CA	2.42	0.46
1:B:4:ILE:CG2	1:B:30:LYS:H	2.25	0.46
1:B:80:ARG:HG2	3:Q:206:ALA:O	2.15	0.46
1:D:63:LEU:HD13	1:D:68:ALA:HB2	1.96	0.46
2:E:28:ALA:N	2:E:87:VAL:HG21	2.31	0.46
2:E:40:GLU:HG2	3:F:210:GLN:HE22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ALA:HB1	1:A:226:ALA:HB2	1.94	0.46
1:B:7:ALA:HA	1:B:62:VAL:HA	1.97	0.46
2:M:88:LEU:O	2:M:92:VAL:N	2.40	0.46
1:C:186:LEU:HD23	1:C:186:LEU:HA	1.75	0.46
1:A:132:ASP:CG	1:A:134:ARG:NE	2.73	0.46
1:B:96:ALA:HB1	1:B:102:ASP:CB	2.46	0.46
2:M:4:MET:SD	3:Q:76:LEU:HD23	2.55	0.46
2:M:83:SER:O	2:M:85:MET:N	2.49	0.46
3:Q:204:LEU:C	3:Q:206:ALA:N	2.73	0.46
1:C:214:ARG:HG3	1:C:215:THR:H	1.81	0.46
1:D:16:GLY:N	1:D:17:GLY:C	2.73	0.46
1:D:123:GLU:OE2	1:D:158:ARG:NH2	2.38	0.46
2:E:59:LYS:O	2:E:60:ILE:HG12	2.15	0.46
2:E:78:VAL:HG13	2:E:127:TYR:CZ	2.51	0.46
3:F:146:LEU:O	3:F:149:TYR:HB3	2.16	0.46
3:Q:2:SER:HA	3:Q:3:ILE:HG23	0.60	0.46
1:C:177:GLU:HG2	1:C:178:GLN:N	2.30	0.46
1:D:137:PRO:HB2	1:D:139:HIS:CE1	2.50	0.46
3:F:242:VAL:C	3:F:244:LEU:N	2.73	0.46
1:A:35:ALA:HB3	1:A:210:VAL:HG22	1.97	0.46
2:E:95:PHE:O	2:E:99:LEU:N	2.38	0.46
3:F:222:ALA:HB1	3:F:226:VAL:CG2	2.46	0.46
1:A:13:ALA:CB	1:A:19:LYS:N	2.72	0.46
1:A:122:GLU:CG	1:A:123:GLU:H	2.24	0.46
1:B:137:PRO:HD2	1:B:140:MET:HE2	1.98	0.46
1:B:263:LEU:HG	1:B:264:PRO:O	2.16	0.46
2:M:90:VAL:HG13	2:M:108:LEU:HD11	1.97	0.46
3:Q:174:THR:CB	3:Q:177:ARG:HG3	2.37	0.46
1:C:244:VAL:HG13	1:C:245:ILE:N	2.30	0.46
1:C:249:LEU:CG	1:C:250:LEU:HD22	2.43	0.46
1:D:13:ALA:CB	1:D:19:LYS:CA	2.84	0.46
1:D:212:LEU:HG	1:D:220:ALA:O	2.16	0.46
1:A:221:GLU:CD	1:A:222:GLY:HA3	2.41	0.46
1:B:44:LYS:H	1:B:44:LYS:HG3	1.44	0.46
2:M:60:ILE:HD13	2:M:60:ILE:HA	1.73	0.46
1:C:129:SER:HB3	1:C:182:LEU:HD11	1.98	0.46
1:D:10:LEU:O	1:D:23:ASP:N	2.49	0.46
2:E:60:ILE:CG2	2:E:61:PRO:O	2.38	0.46
1:A:24:LEU:HD11	1:A:218:VAL:HG22	1.75	0.46
1:A:49:LEU:HB3	1:A:54:THR:HB	1.97	0.46
1:A:158:ARG:N	1:A:159:PRO:HD3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLU:CD	1:A:221:GLU:C	2.84	0.46
3:Q:201:GLU:HG3	3:Q:210:GLN:CD	2.40	0.46
3:Q:227:LEU:C	3:Q:227:LEU:CD1	2.85	0.46
1:C:42:ALA:HB1	1:C:213:PHE:HB3	1.97	0.46
1:C:72:SER:OG	1:C:74:LYS:CG	2.64	0.46
1:C:231:ARG:NH1	1:C:249:LEU:HD23	2.27	0.46
1:D:74:LYS:C	1:D:76:LEU:N	2.73	0.46
1:A:139:HIS:O	1:A:140:MET:HB2	2.15	0.45
1:A:234:LEU:HB3	1:A:239:LEU:O	2.16	0.45
1:A:259:PRO:O	1:A:265:LYS:CD	2.61	0.45
1:B:37:LEU:HD13	1:B:197:THR:HG23	1.98	0.45
1:A:221:GLU:CD	1:A:222:GLY:CA	2.90	0.45
1:B:24:LEU:CD2	1:B:218:VAL:CG1	2.63	0.45
1:B:234:LEU:O	1:B:237:VAL:HG22	2.16	0.45
1:C:124:ALA:C	1:C:126:ALA:H	2.23	0.45
1:D:225:GLU:O	1:D:229:SER:OG	2.18	0.45
1:D:261:ALA:CB	1:D:262:PRO:CD	2.32	0.45
3:F:85:ILE:HG21	3:F:93:GLY:N	2.31	0.45
1:A:83:VAL:CG2	1:A:161:VAL:HB	2.35	0.45
1:A:255:GLY:C	1:A:257:LEU:CD2	2.90	0.45
1:B:63:LEU:CB	1:B:67:THR:O	2.65	0.45
2:M:95:PHE:HB3	2:M:99:LEU:HD12	1.98	0.45
3:Q:66:ALA:O	3:Q:70:VAL:HG22	2.10	0.45
1:C:249:LEU:HD12	1:C:249:LEU:O	2.16	0.45
2:E:6:GLY:O	3:F:109:ALA:HA	2.16	0.45
1:A:85:LEU:HA	1:A:163:LEU:O	2.16	0.45
2:M:172:LEU:C	2:M:172:LEU:CD2	2.85	0.45
3:Q:65:TRP:HA	3:Q:68:VAL:HG23	1.98	0.45
3:Q:205:GLY:O	3:Q:207:ARG:O	2.35	0.45
1:D:199:ASP:OD1	1:D:201:GLU:HB2	2.16	0.45
3:F:84:LEU:CD2	3:F:94:LEU:HD21	2.28	0.45
1:A:12:TYR:C	1:A:12:TYR:CD2	2.95	0.45
1:A:47:LEU:O	1:A:51:LEU:HG	2.16	0.45
1:A:134:ARG:CA	1:A:135:ASP:CB	2.86	0.45
3:Q:3:ILE:HD12	3:Q:3:ILE:O	2.15	0.45
1:C:73:ARG:O	1:C:74:LYS:O	2.32	0.45
2:E:172:LEU:HD12	2:E:172:LEU:O	2.17	0.45
1:A:147:ARG:HH12	1:A:169:ALA:H	1.65	0.45
1:B:24:LEU:HD21	1:B:218:VAL:CB	2.47	0.45
1:B:103:VAL:HG21	1:B:125:LEU:HD21	1.97	0.45
1:B:152:ALA:HA	1:B:155:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:162:MET:HE3	3:Q:192:ARG:HH11	1.61	0.45
1:C:49:LEU:O	1:C:54:THR:N	2.43	0.45
1:D:99:VAL:O	1:D:100:PHE:C	2.59	0.45
2:E:4:MET:SD	3:F:109:ALA:HB1	2.56	0.45
3:F:186:ILE:O	3:F:187:ALA:C	2.58	0.45
3:F:212:GLU:O	3:F:213:MET:HE3	2.16	0.45
1:A:14:PHE:N	1:A:18:VAL:HG22	2.32	0.45
1:B:9:ALA:CB	1:B:10:LEU:O	2.61	0.45
2:M:174:ALA:C	2:M:177:LYS:HG2	2.42	0.45
1:C:248:ALA:O	1:C:251:ALA:HB3	2.16	0.45
1:D:105:PHE:CD1	1:D:105:PHE:O	2.70	0.45
1:D:140:MET:CG	3:F:8:ARG:HH21	2.29	0.45
3:F:124:PRO:O	3:F:125:ALA:C	2.58	0.45
1:A:214:ARG:CZ	1:A:237:VAL:HA	2.46	0.45
1:B:10:LEU:HD12	1:B:11:THR:H	1.81	0.45
1:B:50:HIS:ND1	1:B:55:LEU:O	2.49	0.45
1:B:243:LEU:O	1:B:244:VAL:HG13	2.17	0.45
2:M:74:GLY:HA3	2:M:145:ALA:CB	2.45	0.45
3:Q:15:TRP:CD2	3:Q:58:ALA:HB2	2.52	0.45
1:D:2:THR:HA	1:D:3:PRO:HD3	1.78	0.45
2:E:151:ALA:O	2:E:155:THR:OG1	2.20	0.45
1:B:74:LYS:C	1:B:76:LEU:HD22	2.42	0.45
1:C:234:LEU:HB3	1:C:239:LEU:O	2.16	0.45
1:D:139:HIS:HD2	3:F:153:PHE:CD1	2.34	0.45
1:A:64:LEU:CD1	1:A:67:THR:H	2.25	0.45
2:M:185:THR:C	2:M:188:PRO:HD2	2.42	0.45
1:C:100:PHE:CD2	1:C:121:VAL:HG11	2.52	0.45
1:C:252:ARG:O	1:C:257:LEU:CD1	2.65	0.45
1:D:106:GLY:HA3	1:D:107:PRO:HD3	1.73	0.45
1:D:137:PRO:CG	3:F:16:ARG:HH22	2.30	0.45
1:D:262:PRO:C	1:D:264:PRO:HD3	2.42	0.45
2:E:46:ALA:CB	3:F:151:PHE:CD1	3.00	0.45
2:E:117:ILE:N	2:E:117:ILE:CD1	2.73	0.45
3:F:14:HIS:HD2	3:F:15:TRP:CD1	2.35	0.45
3:F:86:GLN:O	3:F:87:ILE:C	2.59	0.45
1:A:79:TRP:O	1:A:79:TRP:HD1	1.99	0.44
1:A:86:VAL:HG13	1:A:93:GLN:HE22	1.81	0.44
1:A:132:ASP:CG	1:A:134:ARG:HE	2.19	0.44
1:A:225:GLU:CD	1:A:225:GLU:N	2.73	0.44
1:A:256:LEU:N	1:A:257:LEU:HD22	2.32	0.44
1:B:4:ILE:HG21	1:B:30:LYS:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:146:PHE:HD2	2:M:147:LEU:HD23	1.81	0.44
3:Q:170:LEU:C	3:Q:172:HIS:H	2.25	0.44
1:D:28:VAL:HG22	1:D:34:LEU:HD13	1.98	0.44
2:E:44:THR:O	2:E:47:ALA:HB3	2.17	0.44
2:E:111:ASN:N	2:E:111:ASN:ND2	2.60	0.44
1:A:13:ALA:CB	1:A:19:LYS:CA	2.95	0.44
1:A:128:LEU:HD22	1:A:128:LEU:HA	1.81	0.44
1:A:209:ARG:HG3	1:A:209:ARG:NH1	2.30	0.44
1:B:9:ALA:HA	1:B:23:ASP:HB2	2.00	0.44
1:B:114:GLU:OE1	3:Q:216:LEU:HD13	2.17	0.44
3:Q:54:THR:C	3:Q:55:PHE:HD1	2.25	0.44
2:E:23:PHE:HB3	2:E:117:ILE:HG12	1.99	0.44
2:E:192:ALA:O	2:E:195:PHE:N	2.51	0.44
3:F:85:ILE:HG21	3:F:92:ILE:HG23	1.99	0.44
1:A:252:ARG:N	1:A:257:LEU:HG	2.32	0.44
1:B:4:ILE:HA	1:B:65:GLY:HA2	1.98	0.44
2:E:105:LEU:O	2:E:108:LEU:HB3	2.16	0.44
3:F:11:ALA:HB2	3:F:16:ARG:HH12	1.79	0.44
3:F:85:ILE:HG13	3:F:86:GLN:N	2.32	0.44
3:F:200:LEU:HG	3:F:204:LEU:HD13	2.00	0.44
1:A:64:LEU:CD1	1:A:67:THR:N	2.81	0.44
1:A:101:GLU:HA	1:A:101:GLU:OE2	2.15	0.44
1:B:11:THR:CA	1:B:21:LEU:O	2.65	0.44
1:B:13:ALA:HB1	1:B:18:VAL:O	2.18	0.44
1:B:265:LYS:HE3	1:B:266:THR:C	2.42	0.44
3:Q:19:PRO:HD3	3:Q:220:PRO:HG2	1.98	0.44
1:C:231:ARG:CZ	1:C:250:LEU:HD21	2.47	0.44
1:D:49:LEU:HD23	1:D:49:LEU:HA	1.84	0.44
1:B:94:LEU:O	3:Q:150:ARG:NH2	2.50	0.44
1:B:223:ALA:HB1	1:B:225:GLU:HB3	2.00	0.44
1:B:234:LEU:CD2	1:B:239:LEU:C	2.85	0.44
2:M:3:ILE:HG22	2:M:107:THR:HG21	1.99	0.44
2:M:107:THR:O	2:M:110:ALA:HB3	2.18	0.44
2:M:173:GLY:C	2:M:175:ALA:N	2.73	0.44
1:C:263:LEU:CD1	1:C:263:LEU:C	2.86	0.44
1:D:63:LEU:CD1	1:D:68:ALA:CB	2.91	0.44
1:A:15:PRO:CD	1:A:18:VAL:CG2	2.85	0.44
1:A:106:GLY:O	1:A:109:ASN:HB3	2.18	0.44
1:B:11:THR:O	1:B:12:TYR:CB	2.62	0.44
1:B:36:ILE:HG21	1:B:44:LYS:HB3	2.00	0.44
2:M:174:ALA:HA	2:M:177:LYS:CG	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:178:TRP:O	3:Q:178:TRP:CD1	2.70	0.44
1:C:15:PRO:HB2	3:F:5:SER:HA	2.00	0.44
1:D:164:LEU:C	1:D:165:ASP:O	2.57	0.44
1:D:200:VAL:HG23	1:D:242:PRO:HG3	2.00	0.44
2:E:118:VAL:HG11	2:E:155:THR:OG1	2.18	0.44
1:A:147:ARG:CZ	1:A:166:GLU:O	2.65	0.44
2:M:60:ILE:CD1	2:M:196:LEU:HD13	2.44	0.44
3:Q:62:LEU:C	3:Q:64:PHE:N	2.64	0.44
3:Q:238:LEU:HD13	3:Q:239:ALA:HA	2.00	0.44
1:D:252:ARG:C	1:D:253:ASP:OD2	2.61	0.44
3:F:132:LEU:CD2	3:F:137:VAL:HG23	2.31	0.44
1:A:64:LEU:HG	1:A:67:THR:O	2.18	0.44
1:B:10:LEU:HD21	1:B:21:LEU:HD21	2.00	0.44
2:M:2:HIS:CE1	2:M:115:MET:SD	3.11	0.44
1:A:8:GLU:HB2	1:A:61:ARG:NE	2.32	0.44
2:M:4:MET:HE3	3:Q:75:PHE:HD2	1.82	0.44
3:Q:133:ARG:NH2	3:Q:219:ARG:NH2	2.66	0.44
1:C:73:ARG:C	1:C:75:ASP:N	2.74	0.44
1:D:95:PHE:CE1	1:D:105:PHE:HD2	2.36	0.44
1:D:240:ARG:HE	1:D:240:ARG:HB2	1.59	0.44
2:E:42:ARG:CZ	3:F:143:GLU:OE1	2.66	0.44
2:E:152:THR:OG1	2:E:153:TYR:N	2.50	0.44
3:F:205:GLY:O	3:F:208:ASN:N	2.51	0.44
1:A:133:LEU:CA	1:A:134:ARG:HB2	2.48	0.43
2:M:142:PHE:HD1	2:M:194:GLY:C	2.26	0.43
3:Q:65:TRP:O	3:Q:67:SER:N	2.52	0.43
1:C:104:SER:O	1:C:108:LEU:HD13	2.18	0.43
1:D:144:GLY:O	1:D:148:ARG:HG3	2.19	0.43
1:D:224:ALA:O	1:D:228:LEU:N	2.41	0.43
2:E:116:ALA:C	2:E:117:ILE:HD12	2.43	0.43
1:A:119:ALA:HA	1:A:122:GLU:HB3	2.00	0.43
1:A:129:SER:O	1:A:129:SER:OG	2.31	0.43
1:A:255:GLY:CA	1:A:257:LEU:CG	2.95	0.43
1:B:76:LEU:CD2	1:B:77:THR:H	2.31	0.43
1:B:76:LEU:HD23	1:B:77:THR:N	2.32	0.43
3:Q:174:THR:CG2	3:Q:177:ARG:HD3	2.37	0.43
1:C:249:LEU:C	1:C:249:LEU:CD1	2.85	0.43
3:F:84:LEU:HD21	3:F:94:LEU:HG	2.00	0.43
3:F:105:LEU:HD12	3:F:105:LEU:HA	1.57	0.43
1:A:164:LEU:O	1:A:195:PHE:HA	2.18	0.43
1:A:256:LEU:C	1:A:256:LEU:HD22	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:VAL:CG1	1:B:79:TRP:HH2	2.26	0.43
1:B:72:SER:O	1:B:73:ARG:HG2	2.18	0.43
1:B:109:ASN:HD22	3:Q:209:TRP:CB	2.31	0.43
1:B:231:ARG:O	1:B:234:LEU:HB3	2.18	0.43
3:Q:70:VAL:HA	3:Q:73:LEU:HD13	2.00	0.43
1:C:85:LEU:HD12	1:C:163:LEU:HB2	1.99	0.43
1:C:252:ARG:HE	1:C:257:LEU:CB	2.28	0.43
1:D:17:GLY:C	1:D:18:VAL:CG1	2.90	0.43
1:D:214:ARG:HD2	1:D:215:THR:HG23	2.00	0.43
1:D:264:PRO:HB2	1:D:265:LYS:H	1.65	0.43
2:E:71:THR:O	2:E:193:GLU:OE1	2.36	0.43
3:F:82:VAL:HG23	3:F:83:LEU:N	2.29	0.43
3:F:192:ARG:HE	3:F:192:ARG:HB3	1.68	0.43
3:F:210:GLN:HG2	3:F:211:GLY:H	1.83	0.43
3:Q:237:ILE:O	3:Q:237:ILE:HG22	2.17	0.43
1:C:64:LEU:CD2	1:C:82:ARG:HH12	2.32	0.43
1:C:72:SER:OG	1:C:74:LYS:CB	2.66	0.43
1:D:75:ASP:OD1	1:D:75:ASP:N	2.52	0.43
2:E:51:PHE:HE1	3:F:186:ILE:HG23	1.83	0.43
1:B:135:ASP:OD1	1:B:135:ASP:N	2.52	0.43
1:B:247:LEU:CG	1:B:249:LEU:HD23	2.41	0.43
2:M:164:TYR:O	2:M:165:PRO:C	2.58	0.43
3:Q:23:LYS:HZ1	3:Q:122:THR:C	2.21	0.43
1:C:140:MET:O	1:C:140:MET:HG2	2.18	0.43
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.66	0.43
1:C:230:ASP:OD2	1:C:233:THR:OG1	2.31	0.43
1:C:247:LEU:HA	1:C:247:LEU:HD13	1.79	0.43
1:D:252:ARG:HA	1:D:252:ARG:HD2	1.68	0.43
2:E:116:ALA:CB	2:E:117:ILE:CA	2.87	0.43
3:F:97:ASP:HB2	3:F:98:GLY:CA	2.42	0.43
3:F:155:LEU:CD2	3:F:189:LEU:HD11	2.48	0.43
3:F:176:ARG:CG	3:F:177:ARG:H	2.31	0.43
3:F:176:ARG:CG	3:F:177:ARG:N	2.81	0.43
3:F:225:ARG:O	3:F:229:LEU:N	2.41	0.43
1:A:76:LEU:O	1:A:78:GLY:N	2.51	0.43
1:A:112:LEU:HD13	1:A:112:LEU:HA	1.87	0.43
1:B:6:ALA:O	1:B:63:LEU:CD2	2.60	0.43
1:B:18:VAL:HG22	1:B:19:LYS:HG2	1.99	0.43
1:B:240:ARG:HG2	1:B:241:PRO:HD2	2.00	0.43
2:M:16:TRP:CZ2	2:M:159:GLN:HG2	2.54	0.43
2:M:107:THR:O	2:M:110:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:170:LEU:O	3:Q:171:GLY:C	2.62	0.43
1:C:120:ARG:NH1	1:C:120:ARG:CG	2.73	0.43
1:C:209:ARG:NH1	1:C:221:GLU:OE2	2.52	0.43
1:B:24:LEU:HD23	1:B:217:ARG:CB	2.40	0.43
1:B:98:THR:HA	1:B:137:PRO:HA	2.01	0.43
3:Q:37:VAL:O	3:Q:108:ARG:NH2	2.46	0.43
2:E:32:ARG:HD3	3:F:140:GLU:OE2	2.19	0.43
2:E:104:GLY:O	2:E:108:LEU:HB2	2.19	0.43
1:A:155:VAL:C	1:A:157:MET:H	2.27	0.43
1:B:128:LEU:HD13	1:B:152:ALA:HB2	2.00	0.43
2:M:41:ALA:C	2:M:43:MET:H	2.26	0.43
2:M:83:SER:C	2:M:85:MET:N	2.74	0.43
3:Q:178:TRP:CD1	3:Q:178:TRP:C	2.97	0.43
1:C:270:LEU:HD23	1:C:270:LEU:HA	1.87	0.43
3:F:239:ALA:O	3:F:243:LEU:HD23	2.19	0.43
1:A:15:PRO:CD	1:A:18:VAL:H	2.32	0.43
1:A:110:LEU:C	1:A:112:LEU:N	2.77	0.43
1:A:259:PRO:O	1:A:259:PRO:HD2	2.19	0.43
1:B:100:PHE:CE1	1:B:134:ARG:NH2	2.87	0.43
1:B:109:ASN:O	3:Q:208:ASN:ND2	2.39	0.43
2:M:201:VAL:O	2:M:201:VAL:HG12	2.19	0.43
3:Q:116:LEU:HD12	3:Q:116:LEU:HA	1.79	0.43
1:C:268:ASP:OD1	1:D:253:ASP:OD2	2.36	0.43
1:D:24:LEU:HD12	1:D:216:GLY:O	2.17	0.43
1:D:49:LEU:HD22	1:D:54:THR:HG21	2.01	0.43
3:F:143:GLU:OE1	3:F:212:GLU:HA	2.18	0.43
3:F:208:ASN:N	3:F:208:ASN:OD1	2.50	0.43
1:A:221:GLU:CD	1:A:222:GLY:N	2.77	0.43
1:B:177:GLU:HA	1:B:180:LEU:HD12	2.01	0.43
1:B:200:VAL:HG11	1:B:239:LEU:HG	2.01	0.43
2:M:75:LEU:CD2	2:M:200:VAL:HG11	2.49	0.43
1:C:12:TYR:CE2	1:C:14:PHE:CD1	3.07	0.43
1:C:28:VAL:HG22	1:C:34:LEU:HD23	2.01	0.43
1:D:105:PHE:CD1	1:D:105:PHE:C	2.96	0.43
2:E:166:ASP:OD2	2:E:177:LYS:HE3	2.19	0.43
3:F:33:LEU:O	3:F:37:VAL:HB	2.19	0.43
1:B:40:ASN:OD1	1:B:41:GLY:N	2.30	0.42
1:B:179:LEU:O	1:B:182:LEU:N	2.52	0.42
2:M:82:PRO:CG	2:M:124:PHE:CD2	3.02	0.42
2:M:155:THR:O	2:M:159:GLN:HG3	2.19	0.42
3:Q:2:SER:CA	3:Q:3:ILE:CB	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:VAL:HG23	1:C:19:LYS:N	2.34	0.42
2:E:160:LEU:HD23	2:E:160:LEU:HA	1.88	0.42
3:F:15:TRP:CD1	3:F:18:ARG:HD3	2.54	0.42
1:A:10:LEU:HG	1:A:23:ASP:N	2.34	0.42
1:A:76:LEU:HD12	1:A:77:THR:CA	2.48	0.42
1:A:100:PHE:O	1:A:101:GLU:C	2.57	0.42
1:A:166:GLU:HA	1:A:167:PRO:HD3	1.84	0.42
1:A:259:PRO:HG2	1:A:265:LYS:CE	2.48	0.42
1:B:123:GLU:CD	1:B:158:ARG:NH1	2.78	0.42
2:M:5:GLU:HB3	3:Q:113:THR:OG1	2.20	0.42
2:M:74:GLY:O	2:M:77:ALA:HB3	2.19	0.42
3:Q:170:LEU:C	3:Q:172:HIS:N	2.75	0.42
3:Q:170:LEU:HD22	3:Q:170:LEU:HA	1.61	0.42
1:C:42:ALA:CB	1:C:213:PHE:HB3	2.49	0.42
1:C:114:GLU:O	1:C:117:ALA:HB3	2.19	0.42
2:E:5:GLU:HA	2:E:107:THR:HG23	2.01	0.42
2:E:94:LEU:HD23	2:E:94:LEU:HA	1.89	0.42
2:E:114:SER:OG	2:E:115:MET:HG2	2.18	0.42
3:Q:52:ALA:O	3:Q:56:LEU:N	2.40	0.42
1:D:70:GLY:C	1:D:75:ASP:CB	2.92	0.42
1:D:140:MET:HG3	3:F:8:ARG:HH21	1.83	0.42
2:E:2:HIS:ND1	2:E:115:MET:HE1	2.34	0.42
1:A:162:LEU:HD12	1:A:162:LEU:HA	1.91	0.42
1:B:265:LYS:HD2	1:B:265:LYS:C	2.44	0.42
2:M:35:VAL:HG22	2:M:41:ALA:HB3	2.00	0.42
1:D:75:ASP:O	1:D:79:TRP:CB	2.67	0.42
2:E:3:ILE:HD12	2:E:111:ASN:ND2	2.34	0.42
1:A:136:ARG:HE	1:A:141:LEU:HG	1.84	0.42
1:A:168:THR:OG1	1:A:202:LEU:HD22	2.20	0.42
1:B:219:LEU:C	1:B:219:LEU:HD12	2.45	0.42
3:Q:179:LEU:HD12	3:Q:179:LEU:HA	1.85	0.42
3:Q:192:ARG:HE	3:Q:192:ARG:HB2	1.67	0.42
1:C:128:LEU:HD22	1:C:148:ARG:O	2.19	0.42
1:B:8:GLU:O	1:B:9:ALA:C	2.63	0.42
2:M:160:LEU:HD23	2:M:160:LEU:HA	1.80	0.42
1:C:127:ALA:O	1:C:182:LEU:HD22	2.20	0.42
1:D:71:HIS:C	1:D:73:ARG:HA	2.38	0.42
1:D:138:THR:HA	1:D:141:LEU:CD1	2.48	0.42
1:D:256:LEU:CD1	1:D:257:LEU:HD23	2.47	0.42
1:D:267:ARG:NE	1:D:267:ARG:O	2.53	0.42
3:F:125:ALA:O	3:F:129:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:137:VAL:HA	3:F:138:PRO:HD3	1.93	0.42
1:B:82:ARG:HE	1:B:82:ARG:HB3	1.62	0.42
1:B:138:THR:HA	1:B:141:LEU:HD12	2.00	0.42
1:C:21:LEU:HD11	1:C:50:HIS:HD2	1.83	0.42
1:D:151:ILE:O	1:D:155:VAL:HG13	2.20	0.42
2:E:7:TYR:O	2:E:7:TYR:CD2	2.73	0.42
2:E:42:ARG:NH1	3:F:211:GLY:C	2.78	0.42
2:E:113:PHE:O	2:E:118:VAL:HG23	2.19	0.42
1:A:14:PHE:CB	1:A:18:VAL:HG22	2.46	0.42
1:A:115:ALA:C	1:A:118:ARG:HB3	2.45	0.42
1:A:132:ASP:HB3	1:A:133:LEU:CB	2.49	0.42
1:A:247:LEU:HA	1:A:247:LEU:HD13	1.79	0.42
1:B:243:LEU:HD23	1:B:243:LEU:H	1.84	0.42
3:Q:37:VAL:HG11	3:Q:42:GLY:CA	2.45	0.42
3:Q:189:LEU:HD12	3:Q:189:LEU:HA	1.89	0.42
1:C:176:THR:HG23	1:C:177:GLU:N	2.34	0.42
1:C:252:ARG:CG	1:C:257:LEU:HA	2.46	0.42
1:C:252:ARG:NE	1:C:257:LEU:CB	2.71	0.42
1:D:245:ILE:O	1:D:249:LEU:HG	2.20	0.42
2:E:182:PHE:HE1	3:F:78:THR:HG21	1.84	0.42
3:F:15:TRP:CH2	3:F:57:GLY:HA3	2.55	0.42
3:F:82:VAL:CG2	3:F:83:LEU:N	2.83	0.42
1:B:62:VAL:HG12	1:B:79:TRP:HH2	1.85	0.42
1:B:265:LYS:HD2	1:B:267:ARG:CA	2.48	0.42
2:M:54:VAL:O	2:M:58:LEU:HD13	2.20	0.42
2:M:120:PRO:O	2:M:121:TRP:C	2.62	0.42
1:C:17:GLY:C	1:C:19:LYS:N	2.72	0.42
1:C:35:ALA:HB2	1:C:207:ALA:HB2	2.02	0.42
1:C:64:LEU:HD21	1:C:82:ARG:HH12	1.84	0.42
2:E:51:PHE:CE1	3:F:186:ILE:HG23	2.55	0.42
3:F:212:GLU:O	3:F:213:MET:HE2	2.17	0.42
1:A:102:ASP:C	3:Q:169:ARG:HH12	2.27	0.42
1:A:115:ALA:O	1:A:118:ARG:HB3	2.20	0.42
1:A:224:ALA:O	1:A:228:LEU:HD12	2.20	0.42
3:Q:233:LEU:O	3:Q:236:ALA:HB3	2.19	0.42
1:C:186:LEU:O	1:C:189:ALA:N	2.53	0.42
1:D:39:PRO:O	1:D:44:LYS:NZ	2.52	0.42
1:D:98:THR:OG1	1:D:135:ASP:C	2.63	0.42
1:D:207:ALA:O	1:D:224:ALA:HB2	2.19	0.42
1:D:243:LEU:HD23	1:D:243:LEU:C	2.37	0.42
1:D:252:ARG:O	1:D:253:ASP:CG	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:19:ALA:O	2:E:113:PHE:HE1	2.03	0.42
1:A:62:VAL:CG1	1:A:63:LEU:H	2.15	0.41
1:A:259:PRO:CG	1:A:265:LYS:NZ	2.74	0.41
1:B:18:VAL:CG2	1:B:19:LYS:HG2	2.50	0.41
1:B:148:ARG:NH2	1:B:178:GLN:HE22	2.18	0.41
2:M:146:PHE:HD1	2:M:190:ALA:O	2.02	0.41
3:Q:62:LEU:CB	3:Q:64:PHE:HB2	2.44	0.41
1:C:109:ASN:HB3	3:F:170:LEU:HB2	2.02	0.41
1:D:186:LEU:HD23	1:D:186:LEU:HA	1.86	0.41
3:F:66:ALA:O	3:F:70:VAL:HG23	2.20	0.41
1:A:78:GLY:O	1:A:81:ARG:HB3	2.20	0.41
1:B:12:TYR:O	1:B:20:ALA:HB3	2.17	0.41
1:B:120:ARG:NH2	1:B:158:ARG:CZ	2.64	0.41
1:B:243:LEU:CD2	1:B:243:LEU:H	2.34	0.41
2:E:108:LEU:C	2:E:108:LEU:CD2	2.85	0.41
3:F:116:LEU:CD1	3:F:117:LEU:HD12	2.49	0.41
1:B:10:LEU:HD12	1:B:11:THR:N	2.35	0.41
1:B:200:VAL:CG1	1:B:239:LEU:HG	2.51	0.41
2:M:71:THR:C	2:M:73:THR:N	2.78	0.41
2:M:114:SER:HA	2:M:118:VAL:HB	2.02	0.41
3:Q:69:ALA:O	3:Q:72:PRO:CD	2.63	0.41
3:Q:141:LEU:N	3:Q:141:LEU:HD23	2.35	0.41
3:Q:170:LEU:HD13	3:Q:172:HIS:N	2.30	0.41
2:E:55:LEU:HD12	3:F:186:ILE:HD13	2.02	0.41
3:F:15:TRP:HB3	3:F:18:ARG:HB2	2.03	0.41
3:F:51:LEU:CD2	3:F:51:LEU:N	2.83	0.41
3:F:172:HIS:CE1	3:F:178:TRP:HE1	2.38	0.41
1:A:251:ALA:O	1:A:255:GLY:HA3	2.20	0.41
1:B:19:LYS:H	1:B:19:LYS:HG2	1.55	0.41
1:B:157:MET:O	1:B:159:PRO:HD3	2.20	0.41
2:M:61:PRO:HG2	3:Q:179:LEU:HB2	2.02	0.41
2:M:152:THR:OG1	2:M:153:TYR:N	2.52	0.41
3:Q:78:THR:O	3:Q:82:VAL:HG23	2.20	0.41
3:Q:176:ARG:CG	3:Q:176:ARG:NH1	2.79	0.41
1:C:61:ARG:HE	1:C:61:ARG:HB2	1.67	0.41
1:C:212:LEU:HD23	1:C:237:VAL:HG21	2.02	0.41
1:C:252:ARG:C	1:C:254:HIS:N	2.77	0.41
1:D:16:GLY:N	1:D:18:VAL:HG12	2.34	0.41
1:D:16:GLY:HA3	1:D:18:VAL:HB	2.03	0.41
1:D:48:LEU:HD22	1:D:163:LEU:HB3	2.02	0.41
1:D:92:ASP:CG	3:F:199:ARG:HH21	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:MET:CG	3:F:8:ARG:HE	2.34	0.41
2:E:75:LEU:O	2:E:76:GLY:C	2.61	0.41
3:F:151:PHE:O	3:F:155:LEU:HD12	2.19	0.41
3:F:238:LEU:C	3:F:238:LEU:HD12	2.46	0.41
1:B:44:LYS:NZ	1:B:197:THR:O	2.50	0.41
1:D:28:VAL:HG22	1:D:34:LEU:CD1	2.50	0.41
1:D:127:ALA:O	1:D:182:LEU:HD22	2.20	0.41
1:D:249:LEU:HD23	1:D:249:LEU:HA	1.93	0.41
2:E:2:HIS:ND1	2:E:115:MET:CE	2.83	0.41
1:A:15:PRO:HD2	1:A:18:VAL:CG1	2.40	0.41
1:A:180:LEU:HD21	1:A:206:LEU:HB2	2.03	0.41
1:A:213:PHE:HE1	1:A:216:GLY:CA	2.34	0.41
1:B:49:LEU:O	1:B:54:THR:HB	2.20	0.41
1:B:64:LEU:CD2	1:B:64:LEU:N	2.73	0.41
1:D:163:LEU:HD23	1:D:194:VAL:HB	2.01	0.41
2:E:33:LYS:O	2:E:35:VAL:N	2.53	0.41
2:E:40:GLU:O	2:E:41:ALA:C	2.64	0.41
3:F:105:LEU:O	3:F:108:ARG:N	2.53	0.41
1:A:131:SER:O	1:A:132:ASP:CB	2.60	0.41
1:A:166:GLU:HG3	1:A:197:THR:HA	2.01	0.41
1:B:37:LEU:HD12	1:B:38:GLY:H	1.85	0.41
1:B:138:THR:C	1:B:140:MET:N	2.73	0.41
1:D:265:LYS:C	1:D:266:THR:HG1	2.19	0.41
2:E:60:ILE:HG23	2:E:61:PRO:HD2	2.02	0.41
3:F:85:ILE:CG2	3:F:92:ILE:O	2.66	0.41
1:B:4:ILE:O	1:B:65:GLY:N	2.46	0.41
1:B:64:LEU:CD2	1:B:64:LEU:O	2.68	0.41
1:B:163:LEU:C	1:B:164:LEU:HD12	2.46	0.41
1:B:265:LYS:HE3	1:B:266:THR:O	2.21	0.41
2:M:90:VAL:O	2:M:94:LEU:HG	2.21	0.41
3:Q:2:SER:CB	3:Q:3:ILE:CG1	2.96	0.41
3:Q:65:TRP:HZ3	3:Q:117:LEU:CB	2.33	0.41
3:Q:87:ILE:HG22	3:Q:88:GLY:CA	2.51	0.41
1:C:53:GLY:HA3	1:C:79:TRP:CZ3	2.55	0.41
1:C:77:THR:O	1:C:81:ARG:N	2.54	0.41
1:C:120:ARG:HD3	1:C:156:ALA:O	2.21	0.41
1:C:162:LEU:HD23	1:C:164:LEU:HD11	2.02	0.41
1:D:90:ALA:O	1:D:94:LEU:HG	2.21	0.41
1:D:97:THR:HG21	3:F:126:ALA:HB3	2.02	0.41
2:E:195:PHE:O	2:E:199:ILE:HG13	2.20	0.41
1:A:24:LEU:HB2	1:A:217:ARG:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:PHE:HD1	1:A:100:PHE:HA	1.72	0.41
1:A:120:ARG:C	1:A:122:GLU:N	2.79	0.41
1:A:161:VAL:HG22	1:A:192:THR:HB	2.02	0.41
1:B:34:LEU:HA	1:B:209:ARG:O	2.20	0.41
2:M:95:PHE:O	2:M:99:LEU:HB2	2.21	0.41
2:M:193:GLU:O	2:M:197:THR:HG23	2.21	0.41
3:Q:2:SER:CA	3:Q:3:ILE:CG2	2.42	0.41
3:Q:15:TRP:CZ2	3:Q:57:GLY:O	2.74	0.41
3:Q:50:ILE:HG23	3:Q:51:LEU:HD23	2.03	0.41
3:Q:91:GLY:C	3:Q:92:ILE:CG2	2.93	0.41
1:C:112:LEU:O	1:C:113:SER:CB	2.69	0.41
1:D:7:ALA:HB2	1:D:62:VAL:HG22	2.01	0.41
1:D:212:LEU:HD11	1:D:234:LEU:CD2	2.50	0.41
2:E:5:GLU:HA	2:E:107:THR:HG21	2.03	0.41
3:F:71:LEU:HD13	3:F:74:GLY:CA	2.48	0.41
1:A:121:VAL:O	1:A:121:VAL:HG12	2.21	0.41
1:B:45:SER:OG	1:B:88:GLN:NE2	2.54	0.41
2:M:128:LYS:HG2	2:M:129:LEU:HD12	2.02	0.41
2:M:173:GLY:C	2:M:175:ALA:H	2.29	0.41
3:Q:224:ALA:HA	3:Q:227:LEU:HB3	2.02	0.41
1:C:214:ARG:C	1:C:216:GLY:N	2.79	0.41
1:C:231:ARG:NH1	1:C:246:ASP:OD2	2.54	0.41
2:E:92:VAL:O	2:E:96:GLN:HG3	2.21	0.41
3:F:22:GLU:HG3	3:F:222:ALA:HB3	1.98	0.41
3:F:42:GLY:O	3:F:45:LEU:HD13	2.19	0.41
3:F:242:VAL:HG13	3:F:243:LEU:H	1.86	0.41
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.80	0.40
1:B:224:ALA:O	1:B:228:LEU:CD2	2.68	0.40
1:D:138:THR:OG1	3:F:150:ARG:NH1	2.54	0.40
1:D:224:ALA:HB3	1:D:225:GLU:OE2	2.21	0.40
1:D:243:LEU:HD23	1:D:244:VAL:CG2	2.50	0.40
3:F:159:ALA:HA	3:F:162:MET:HE3	2.03	0.40
1:A:213:PHE:CE1	1:A:216:GLY:C	2.86	0.40
1:B:91:ASP:OD1	1:B:146:LYS:NZ	2.45	0.40
2:M:53:PHE:CD2	2:M:53:PHE:C	3.00	0.40
3:Q:85:ILE:HD12	3:Q:86:GLN:HE21	1.79	0.40
3:Q:221:PRO:O	3:Q:223:SER:N	2.54	0.40
3:Q:224:ALA:HB1	3:Q:227:LEU:HD23	2.03	0.40
1:D:87:LEU:HD11	3:F:203:GLY:HA2	2.02	0.40
3:F:223:SER:O	3:F:224:ALA:C	2.64	0.40
1:A:251:ALA:C	1:A:257:LEU:HG	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:PRO:HG2	1:A:265:LYS:HZ3	1.84	0.40
1:B:8:GLU:O	1:B:10:LEU:N	2.55	0.40
1:B:24:LEU:CD1	1:B:24:LEU:C	2.94	0.40
1:B:36:ILE:HG23	1:B:213:PHE:CE2	2.56	0.40
1:B:214:ARG:O	1:B:215:THR:CB	2.70	0.40
2:M:41:ALA:C	2:M:43:MET:N	2.78	0.40
2:M:160:LEU:HB3	2:M:178:PHE:CE2	2.56	0.40
2:M:187:ILE:O	2:M:187:ILE:HG22	2.21	0.40
3:F:150:ARG:HG2	3:F:154:ILE:CD1	2.51	0.40
3:F:192:ARG:O	3:F:196:ARG:HB2	2.20	0.40
3:F:225:ARG:HH11	3:F:225:ARG:HG2	1.87	0.40
1:B:70:GLY:H	1:B:75:ASP:CG	2.25	0.40
1:B:103:VAL:HG21	1:B:125:LEU:CD2	2.52	0.40
1:B:129:SER:O	1:B:129:SER:OG	2.37	0.40
2:M:64:THR:HG22	2:M:188:PRO:CG	2.51	0.40
3:Q:233:LEU:C	3:Q:233:LEU:CD2	2.85	0.40
1:C:162:LEU:HD23	1:C:193:LEU:HD22	2.04	0.40
1:C:177:GLU:OE1	1:C:178:GLN:HB2	2.22	0.40
1:D:5:LEU:HD13	1:D:64:LEU:HD12	2.04	0.40
1:D:37:LEU:HD11	1:D:239:LEU:CD1	2.52	0.40
1:D:171:LEU:HA	1:D:171:LEU:HD23	1.88	0.40
2:E:7:TYR:CE1	3:F:105:LEU:HD21	2.57	0.40
2:E:27:GLY:C	2:E:87:VAL:HG21	2.47	0.40
3:F:50:ILE:HA	3:F:50:ILE:HD12	1.82	0.40
1:A:154:ALA:HB1	1:A:162:LEU:HD11	2.02	0.40
1:B:231:ARG:HD2	1:B:241:PRO:HD3	2.03	0.40
1:D:250:LEU:C	1:D:252:ARG:N	2.80	0.40
2:E:127:TYR:HE2	2:E:141:VAL:HG12	1.87	0.40
3:F:118:PHE:CE1	3:F:122:THR:HG21	2.57	0.40
3:F:176:ARG:C	3:F:178:TRP:H	2.28	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:SER:CB	1:A:254:HIS:CE1[4_479]	1.33	0.87
1:B:251:ALA:CB	3:F:100:ALA:CB[2_374]	1.51	0.69
1:A:113:SER:OG	1:A:254:HIS:NE2[4_479]	1.58	0.62
1:A:113:SER:OG	1:A:254:HIS:CE1[4_479]	1.66	0.54
1:A:113:SER:CB	1:A:254:HIS:NE2[4_479]	2.02	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:243:LEU:C	3:F:225:ARG:NH1[3_459]	2.08	0.12
1:B:61:ARG:NH1	3:F:212:GLU:OE2[4_569]	2.11	0.09
3:Q:243:LEU:CA	3:F:225:ARG:CZ[3_459]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	259/280 (92%)	206 (80%)	36 (14%)	17 (7%)	1	11
1	B	254/280 (91%)	202 (80%)	38 (15%)	14 (6%)	1	13
1	C	268/280 (96%)	224 (84%)	32 (12%)	12 (4%)	2	17
1	D	265/280 (95%)	221 (83%)	33 (12%)	11 (4%)	2	18
2	E	205/222 (92%)	160 (78%)	39 (19%)	6 (3%)	3	26
2	M	205/222 (92%)	176 (86%)	20 (10%)	9 (4%)	2	17
3	F	242/256 (94%)	186 (77%)	42 (17%)	14 (6%)	1	12
3	Q	241/256 (94%)	182 (76%)	40 (17%)	19 (8%)	1	8
All	All	1939/2076 (93%)	1557 (80%)	280 (14%)	102 (5%)	1	14

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	LEU
1	A	114	GLU
1	A	140	MET
1	A	145	GLN
1	A	243	LEU
1	B	9	ALA
1	B	22	ASP
1	B	30	LYS
1	B	71	HIS

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Mol	Chain	Res	Type
1	B	72	SER
2	M	165	PRO
3	Q	3	ILE
3	Q	91	GLY
3	Q	168	ALA
3	Q	169	ARG
3	Q	238	LEU
3	Q	239	ALA
1	C	14	PHE
1	C	91	ASP
1	C	112	LEU
1	C	243	LEU
1	C	269	ALA
1	D	250	LEU
1	D	264	PRO
2	E	66	SER
2	E	134	GLY
3	F	87	ILE
3	F	213	MET
3	F	237	ILE
3	F	238	LEU
1	A	144	GLY
1	A	266	THR
1	B	12	TYR
1	B	113	SER
1	B	264	PRO
2	M	172	LEU
2	M	175	ALA
3	Q	73	LEU
3	Q	213	MET
3	Q	222	ALA
3	Q	224	ALA
1	C	113	SER
1	C	125	LEU
1	C	259	PRO
1	C	267	ARG
1	D	261	ALA
1	D	262	PRO
3	F	40	PHE
3	F	84	LEU
3	F	224	ALA
1	A	14	PHE

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Mol	Chain	Res	Type
1	A	15	PRO
1	A	62	VAL
1	A	134	ARG
1	A	135	ASP
1	A	259	PRO
1	B	215	THR
2	M	171	PHE
3	Q	125	ALA
3	Q	182	THR
3	Q	227	LEU
1	C	215	THR
1	D	14	PHE
1	D	18	VAL
1	D	71	HIS
1	D	167	PRO
1	D	265	LYS
3	F	94	LEU
1	A	137	PRO
1	A	206	LEU
1	B	11	THR
1	B	244	VAL
1	B	262	PRO
1	B	265	LYS
2	M	112	ALA
3	Q	12	GLN
3	F	41	PRO
3	F	96	PRO
1	A	143	GLY
2	M	84	VAL
2	M	173	GLY
3	Q	87	ILE
3	Q	221	PRO
3	Q	236	ALA
1	C	216	GLY
1	D	99	VAL
1	D	263	LEU
3	F	99	PRO
1	B	29	PRO
3	Q	96	PRO
2	E	65	GLY
3	F	71	LEU
3	F	98	GLY

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Mol	Chain	Res	Type
1	A	258	ALA
2	M	39	PRO
2	M	70	PRO
1	C	18	VAL
2	E	34	ILE
2	E	90	VAL
3	F	191	PRO
3	Q	237	ILE
2	E	167	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/209 (94%)	136 (69%)	61 (31%)	0	2
1	B	194/209 (93%)	149 (77%)	45 (23%)	1	5
1	C	202/209 (97%)	164 (81%)	38 (19%)	1	9
1	D	200/209 (96%)	160 (80%)	40 (20%)	1	7
2	E	143/155 (92%)	115 (80%)	28 (20%)	1	8
2	M	143/155 (92%)	129 (90%)	14 (10%)	7	30
3	F	179/190 (94%)	151 (84%)	28 (16%)	2	15
3	Q	179/190 (94%)	135 (75%)	44 (25%)	1	4
All	All	1437/1526 (94%)	1139 (79%)	298 (21%)	1	6

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	11	THR
1	A	12	TYR
1	A	19	LYS
1	A	21	LEU
1	A	24	LEU

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Mol	Chain	Res	Type
1	A	30	LYS
1	A	36	ILE
1	A	46	THR
1	A	50	HIS
1	A	52	ASN
1	A	56	ARG
1	A	61	ARG
1	A	64	LEU
1	A	82	ARG
1	A	98	THR
1	A	99	VAL
1	A	100	PHE
1	A	102	ASP
1	A	104	SER
1	A	105	PHE
1	A	107	PRO
1	A	110	LEU
1	A	112	LEU
1	A	114	GLU
1	A	123	GLU
1	A	128	LEU
1	A	131	SER
1	A	132	ASP
1	A	133	LEU
1	A	134	ARG
1	A	136	ARG
1	A	138	THR
1	A	140	MET
1	A	141	LEU
1	A	145	GLN
1	A	158	ARG
1	A	166	GLU
1	A	172	ASP
1	A	178	GLN
1	A	183	LEU
1	A	186	LEU
1	A	208	ASP
1	A	214	ARG
1	A	217	ARG
1	A	221	GLU
1	A	231	ARG
1	A	233	THR

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Mol	Chain	Res	Type
1	A	237	VAL
1	A	245	ILE
1	A	246	ASP
1	A	247	LEU
1	A	249	LEU
1	A	250	LEU
1	A	252	ARG
1	A	256	LEU
1	A	257	LEU
1	A	260	GLU
1	A	263	LEU
1	A	265	LYS
1	A	266	THR
1	B	4	ILE
1	B	8	GLU
1	B	10	LEU
1	B	11	THR
1	B	15	PRO
1	B	18	VAL
1	B	19	LYS
1	B	23	ASP
1	B	24	LEU
1	B	25	SER
1	B	26	LEU
1	B	44	LYS
1	B	61	ARG
1	B	63	LEU
1	B	64	LEU
1	B	69	THR
1	B	71	HIS
1	B	72	SER
1	B	74	LYS
1	B	76	LEU
1	B	81	ARG
1	B	83	VAL
1	B	112	LEU
1	B	114	GLU
1	B	118	ARG
1	B	134	ARG
1	B	136	ARG
1	B	139	HIS
1	B	146	LYS

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Mol	Chain	Res	Type
1	B	158	ARG
1	B	187	ARG
1	B	218	VAL
1	B	229	SER
1	B	231	ARG
1	B	234	LEU
1	B	236	LYS
1	B	239	LEU
1	B	240	ARG
1	B	241	PRO
1	B	243	LEU
1	B	244	VAL
1	B	247	LEU
1	B	249	LEU
1	B	265	LYS
1	B	267	ARG
2	M	8	LEU
2	M	32	ARG
2	M	60	ILE
2	M	67	CYS
2	M	69	HIS
2	M	71	THR
2	M	85	MET
2	M	102	HIS
2	M	108	LEU
2	M	139	VAL
2	M	171	PHE
2	M	172	LEU
2	M	176	LEU
2	M	184	LEU
3	Q	1	MET
3	Q	6	ILE
3	Q	8	ARG
3	Q	18	ARG
3	Q	22	GLU
3	Q	33	LEU
3	Q	36	THR
3	Q	37	VAL
3	Q	40	PHE
3	Q	46	VAL
3	Q	48	VAL
3	Q	51	LEU

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Mol	Chain	Res	Type
3	Q	55	PHE
3	Q	56	LEU
3	Q	59	ARG
3	Q	63	ARG
3	Q	64	PHE
3	Q	68	VAL
3	Q	70	VAL
3	Q	85	ILE
3	Q	90	GLU
3	Q	113	THR
3	Q	132	LEU
3	Q	135	TRP
3	Q	136	ARG
3	Q	141	LEU
3	Q	152	VAL
3	Q	158	GLU
3	Q	163	THR
3	Q	164	THR
3	Q	167	ARG
3	Q	170	LEU
3	Q	176	ARG
3	Q	180	ARG
3	Q	181	SER
3	Q	199	ARG
3	Q	207	ARG
3	Q	208	ASN
3	Q	213	MET
3	Q	223	SER
3	Q	225	ARG
3	Q	227	LEU
3	Q	229	LEU
3	Q	238	LEU
1	C	2	THR
1	C	14	PHE
1	C	19	LYS
1	C	44	LYS
1	C	50	HIS
1	C	56	ARG
1	C	63	LEU
1	C	64	LEU
1	C	67	THR
1	C	73	ARG

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Mol	Chain	Res	Type
1	C	74	LYS
1	C	87	LEU
1	C	89	ASP
1	C	116	GLU
1	C	118	ARG
1	C	128	LEU
1	C	139	HIS
1	C	147	ARG
1	C	158	ARG
1	C	173	LEU
1	C	177	GLU
1	C	178	GLN
1	C	192	THR
1	C	197	THR
1	C	217	ARG
1	C	221	GLU
1	C	229	SER
1	C	237	VAL
1	C	245	ILE
1	C	246	ASP
1	C	247	LEU
1	C	249	LEU
1	C	250	LEU
1	C	253	ASP
1	C	257	LEU
1	C	265	LYS
1	C	266	THR
1	C	270	LEU
1	D	2	THR
1	D	8	GLU
1	D	14	PHE
1	D	15	PRO
1	D	19	LYS
1	D	45	SER
1	D	52	ASN
1	D	59	SER
1	D	63	LEU
1	D	72	SER
1	D	73	ARG
1	D	74	LYS
1	D	75	ASP
1	D	101	GLU

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Mol	Chain	Res	Type
1	D	104	SER
1	D	109	ASN
1	D	114	GLU
1	D	122	GLU
1	D	123	GLU
1	D	129	SER
1	D	131	SER
1	D	139	HIS
1	D	140	MET
1	D	146	LYS
1	D	155	VAL
1	D	166	GLU
1	D	197	THR
1	D	208	ASP
1	D	234	LEU
1	D	242	PRO
1	D	243	LEU
1	D	244	VAL
1	D	247	LEU
1	D	252	ARG
1	D	253	ASP
1	D	256	LEU
1	D	257	LEU
1	D	263	LEU
1	D	265	LYS
1	D	267	ARG
2	E	1	MET
2	E	24	VAL
2	E	29	LEU
2	E	30	LYS
2	E	31	ILE
2	E	32	ARG
2	E	34	ILE
2	E	40	GLU
2	E	42	ARG
2	E	68	SER
2	E	69	HIS
2	E	83	SER
2	E	106	THR
2	E	108	LEU
2	E	111	ASN
2	E	113	PHE

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Mol	Chain	Res	Type
2	E	117	ILE
2	E	120	PRO
2	E	136	SER
2	E	137	MET
2	E	141	VAL
2	E	150	LEU
2	E	152	THR
2	E	162	LEU
2	E	169	SER
2	E	172	LEU
2	E	181	VAL
2	E	200	VAL
3	F	3	ILE
3	F	8	ARG
3	F	31	LEU
3	F	36	THR
3	F	41	PRO
3	F	51	LEU
3	F	53	PHE
3	F	71	LEU
3	F	84	LEU
3	F	85	ILE
3	F	89	PRO
3	F	90	GLU
3	F	92	ILE
3	F	116	LEU
3	F	128	LEU
3	F	133	ARG
3	F	147	LEU
3	F	155	LEU
3	F	167	ARG
3	F	180	ARG
3	F	189	LEU
3	F	199	ARG
3	F	202	THR
3	F	214	ARG
3	F	216	LEU
3	F	218	THR
3	F	225	ARG
3	F	237	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	109	ASN
1	A	139	HIS
1	B	50	HIS
1	B	71	HIS
1	B	88	GLN
1	B	93	GLN
1	B	109	ASN
1	B	198	HIS
2	M	69	HIS
3	Q	86	GLN
3	Q	208	ASN
3	Q	210	GLN
1	C	178	GLN
1	D	40	ASN
1	D	71	HIS
1	D	109	ASN
1	D	139	HIS
2	E	2	HIS
2	E	69	HIS
2	E	96	GLN
2	E	111	ASN
3	F	14	HIS
3	F	172	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	263/280 (93%)	0.97	40 (15%)	5 5	28, 91, 141, 154	0
1	B	258/280 (92%)	0.95	33 (12%)	7 6	56, 80, 111, 132	0
1	C	270/280 (96%)	0.70	19 (7%)	22 15	54, 65, 99, 134	0
1	D	267/280 (95%)	0.56	12 (4%)	38 21	48, 62, 84, 113	0
2	E	207/222 (93%)	0.63	16 (7%)	19 13	53, 62, 81, 116	0
2	M	207/222 (93%)	0.53	12 (5%)	29 17	56, 62, 86, 147	0
3	F	244/256 (95%)	0.67	20 (8%)	17 12	53, 62, 114, 148	0
3	Q	243/256 (94%)	0.62	17 (6%)	22 15	51, 69, 85, 122	0
All	All	1959/2076 (94%)	0.71	169 (8%)	16 11	28, 68, 110, 154	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	211	GLY	9.5
3	Q	86	GLN	6.3
2	E	57	ALA	6.2
3	F	96	PRO	5.9
3	F	83	LEU	5.9
1	B	160	GLU	5.8
1	B	6	ALA	5.6
1	B	194	VAL	5.5
3	F	174	THR	5.3
1	A	142	SER	5.2
1	B	250	LEU	4.5
3	F	93	GLY	4.4
1	A	239	LEU	4.4
1	C	71	HIS	4.4
1	D	165	ASP	4.3
3	F	87	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	193	LEU	4.0
3	F	210	GLN	3.9
1	D	213	PHE	3.9
1	B	33	SER	3.8
1	C	261	ALA	3.7
2	E	165	PRO	3.7
1	C	255	GLY	3.6
1	D	220	ALA	3.6
1	A	141	LEU	3.5
3	F	172	HIS	3.5
1	B	112	LEU	3.5
2	E	100	LEU	3.5
1	B	111	GLY	3.4
3	Q	92	ILE	3.3
1	B	246	ASP	3.3
1	A	262	PRO	3.3
1	A	138	THR	3.3
1	D	62	VAL	3.3
1	A	160	GLU	3.3
3	Q	13	GLY	3.3
1	A	145	GLN	3.2
1	B	216	GLY	3.1
1	A	268	ASP	3.1
1	A	210	VAL	3.0
1	A	244	VAL	3.0
1	A	258	ALA	3.0
1	B	65	GLY	3.0
1	B	218	VAL	3.0
1	D	76	LEU	2.9
3	Q	172	HIS	2.9
1	A	136	ARG	2.9
3	F	117	LEU	2.9
1	B	24	LEU	2.9
1	B	188	ALA	2.9
2	M	205	ALA	2.9
2	M	7	TYR	2.9
1	A	48	LEU	2.8
1	A	190	GLY	2.8
2	E	60	ILE	2.8
3	Q	3	ILE	2.8
1	A	218	VAL	2.8
1	C	75	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	117	ALA	2.8
3	F	94	LEU	2.8
1	A	66	GLY	2.7
2	E	95	PHE	2.7
1	C	216	GLY	2.7
2	E	173	GLY	2.7
2	M	78	VAL	2.7
2	E	58	LEU	2.7
3	Q	41	PRO	2.7
3	F	72	PRO	2.7
1	A	155	VAL	2.7
1	C	257	LEU	2.7
1	C	59	SER	2.7
2	E	101	ALA	2.7
1	C	14	PHE	2.6
1	A	62	VAL	2.6
3	Q	4	ALA	2.6
1	D	34	LEU	2.6
1	D	263	LEU	2.6
3	F	84	LEU	2.6
1	B	4	ILE	2.6
1	B	113	SER	2.6
1	A	137	PRO	2.6
1	D	216	GLY	2.6
2	M	76	GLY	2.6
1	C	97	THR	2.6
3	F	5	SER	2.6
2	E	172	LEU	2.6
2	M	33	LYS	2.6
1	C	45	SER	2.5
2	E	83	SER	2.5
1	C	63	LEU	2.5
1	B	42	ALA	2.5
3	Q	154	ILE	2.5
1	C	251	ALA	2.5
1	D	111	GLY	2.5
3	F	212	GLU	2.4
1	B	189	ALA	2.4
1	A	36	ILE	2.4
1	B	135	ASP	2.4
1	B	5	LEU	2.4
1	A	65	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	241	PRO	2.4
1	B	11	THR	2.4
1	B	137	PRO	2.4
2	M	174	ALA	2.3
1	B	26	LEU	2.3
3	F	17	SER	2.3
3	F	89	PRO	2.3
1	A	235	ALA	2.3
1	D	71	HIS	2.3
2	E	135	ALA	2.3
1	A	219	LEU	2.3
3	F	3	ILE	2.3
1	A	246	ASP	2.3
2	M	6	GLY	2.3
2	M	206	GLY	2.3
1	A	243	LEU	2.3
1	A	263	LEU	2.3
3	F	244	LEU	2.3
1	B	72	SER	2.3
1	B	23	ASP	2.3
1	D	161	VAL	2.3
1	C	42	ALA	2.2
2	E	59	LYS	2.2
3	Q	73	LEU	2.2
3	F	207	ARG	2.2
1	B	244	VAL	2.2
1	C	58	GLN	2.2
1	A	261	ALA	2.2
1	B	171	LEU	2.2
1	B	261	ALA	2.2
3	Q	206	ALA	2.2
2	E	69	HIS	2.2
1	C	12	TYR	2.2
1	C	210	VAL	2.2
1	A	122	GLU	2.2
2	E	4	MET	2.2
3	F	16	ARG	2.2
1	B	183	LEU	2.2
1	A	119	ALA	2.2
2	M	140	ALA	2.2
1	A	161	VAL	2.1
1	B	200	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	Q	188	ALA	2.1
1	C	70	GLY	2.1
3	Q	74	GLY	2.1
1	A	102	ASP	2.1
3	Q	97	ASP	2.1
1	A	47	LEU	2.1
3	Q	210	GLN	2.1
1	C	262	PRO	2.1
1	D	28	VAL	2.1
3	Q	62	LEU	2.1
1	A	39	PRO	2.1
2	M	171	PHE	2.1
2	E	56	SER	2.1
1	A	237	VAL	2.1
2	M	124	PHE	2.1
2	E	29	LEU	2.0
1	A	79	TRP	2.0
3	Q	95	ALA	2.0
1	B	170	GLY	2.0
1	A	200	VAL	2.0
1	B	10	LEU	2.0
1	C	35	ALA	2.0
2	M	116	ALA	2.0
1	A	165	ASP	2.0
3	Q	158	GLU	2.0
1	A	5	LEU	2.0
1	A	133	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.